The Einsteinian T(3)-gauge approach and the stress tensor of the screw dislocation in the second order: avoiding the cut-off at the core

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Abstract

A translational gauge approach of the Einstein type is proposed for obtaining the stresses that are due to non-singular screw dislocation. The stress distribution of second order around the screw dislocation is classically known for the hollow circular cylinder with traction-free external and internal boundaries. The inner boundary surrounds the dislocation's core, which is not captured by the conventional solution. The present gauge approach enables us to continue the classically known quadratic stresses inside the core. The gauge equation is chosen in the Hilbert–Einstein form, and it plays the role of non-conventional incompatibility law. The stress function method is used, and it leads to the modified stress potential given by two constituents: the conventional one, say, the 'background' and a short-ranged gauge contribution. The latter just causes additional stresses, which are localized. The asymptotic properties of the resulting stresses are studied. Since the gauge contributions are short-ranged, the background stress field dominates sufficiently far from the core. The outer cylinder's boundary is traction-free. At sufficiently moderate distances, the second order stresses acquire regular continuation within the core region, and the cut-off at the core does not occur. Expressions for the asymptotically far stresses provide self-consistently new length scales dependent on the elastic parameters. These lengths could characterize an exteriority of the dislocation core region.

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1 Introduction

A model of non-singular screw dislocation is proposed in the present paper. The description is based on the translational gauge approach of the Einstein type. The aim of the paper is to investigate the corresponding stress problem in the second order approximation.

Solutions to the stress problem for the edge and screw dislocations by means of the theoretical elasticity are known both in the linear and quadratic approximations (see [1]– [4]). The stress distributions of the first order are singular on the dislocation lines. Beyond the scope of the linear elasticity, the dislocations have been conventionally considered in [5]– [8] (the non-linear approaches are reviewed in [9] and [10]). The stress solutions provided by [5]– [8] are valid for the hollow cylinders subject to the traction-free conditions on the external and internal boundaries. The corresponding internal radii, as the dislocation core boundaries, remain unspecified. Note that 'core' is rather a crystalline notion since the theoretical elasticity does not have an appropriate length scale.

The relevance of the second order effects in the theoretical elasticity to the lattice modelling of the dislocations has been discussed in [9]. It is not sufficient to use only the linear elasticity for the description of strongly distorted regions of the dislocation cores (see also [3], [4], [9], and [10]). Self-consistency of appropriate boundary-value problems at the dislocation cores also seems theoretically challenging.

The Lagrangian field theory based on the gauge group $T(3) \rtimes SO(3)$ has been proposed in [11] and [12] as a non-conventional approach to the defects in the elastic continua. The Maxwell-type Lagrangian has been proposed to govern the translational gauge potentials. The ordinary screw dislocation, as an asymptotic configuration, is allowed for in [11] and [12]. Owing to the relevance of higher approximations, it has been further attempted in [13] to use [11] for obtaining the corresponding stresses of the second order around the screw dislocation.

An important modification has later been proposed in [14] for the translational gauge equation advanced in [11] and [12]. The modification is concerned with the corresponding driving source. In its new form, it is given by the difference between the stress tensor of the model and the stress due to a classical *background* dislocation. In this particular case, the choice of the background corresponds to the screw dislocation. The linear approach of [14] results in a *modified* screw dislocation, which is equivalent, for sufficiently large distances, to the ordinary one. It is crucial that additional short-ranged stresses, which remove the classical stress singularities, arise. However, it is problematic [15] to obtain analogously a non-singular edge dislocation by means of the translational Lagrangian [11] alone.

Further, the translational gauge approach to the elimination of the dislocation singularities has been developed in [15]– [19]. The driving source of the gauge equations in [15]– [19] is the same as in [14], i.e., it is given in the form of the difference of two stresses. The same modified screw dislocation as in [14] is allowed for in [15] and [17] as well.

Non-local elasticity should be also recalled as a non-gauge opportunity for extending the conventional elasticity framework. Similarly to [14], the singularity-less screw dislocation has already been independently obtained in [20] (see also [21]) by means of the non-local elasticity. Moreover, the first strain gradient elasticity [22]– [27], as well as the generalized elasticity [28]– [30], also admits non-singular solutions for the dislocations.

Let us turn again to the gauge approach [13], where the method of stress functions [5], [7] is used. In principle, the corresponding Kröner ansatz for the screw dislocation, in the second order, is the same as for the edge dislocation, in the first order. However, according to [15], the use of the Maxwell-type translational Lagrangian does not allow for the Airy stress

function with a correct numerical coefficient. Although this Lagrangian is successful for the screw dislocation in the first order, its usage beyond the scope of the linear approximation looks doubtful. Moreover, the elastic energy in [13] does not contain the terms of third order, which are accounted for in [5], [6], and [7]. There is no continuation of the stresses within the core region. Therefore, the experience of [13] looks, to a certain extent, incomplete.

In principle, the translational gauge approaches discussed in refs. [15]–[19] look promising for study in the second order. Indeed, the length scales are "generated" in these models, and the singularities are smoothed out within compact core regions. The active interest in modelling the defects and their cores, as well as the importance of the higher approximations, stimulate us to investigate the gauge models further in order to gain more realistic descriptions of the core regions.

Specifically, ref. [15] is based on the Hilbert–Einstein gauge Lagrangian. Two solutions are found therein, which modify, for short distances, the Airy and Prandtl dislocational stress functions. The stress singularities of both classical dislocations are thus removed. However, certain components of the modified stresses in the "edge" case do not behave properly at infinity.

The approach used in [16]–[19] is based on the Lagrangian quadratic in the $T(3)$-gauge field strength. This quadratic form is based on three gauge-material constants[1] and therefore is different from that in [14]. The inclusion of the terms corresponding to the energy of the rotation gradients enables one to obtain the modified edge dislocation with an appropriate large distance behaviour (see [19]). The model from [19] contains, in general, ten material constants.

The model [15] looks attractive for study in the quadratic approximation. Indeed, the Kröner ansatz for it can be specified, in each order, appropriately. The gauge approach, say, [16]–[19], would require a rather sophisticated choice of the gauge parameters for different orders. The Hilbert–Einsteinian approach implies a single gauge parameter and looks preferable because of the essential non-linearity of descriptions based on it. Besides, the corresponding Einstein tensor is important in the conventional dislocation theory as well.

In the present paper, the model [15] is investigated along the line of [5], [6], and [7]. The background defect is given by the straight screw dislocation in the infinite circular cylinder. Its stress field is taken up to the second-order terms considered in [7]. The Einstein-type gauge equation plays the role of unconventional incompatibility law. The stress function approach is used. The stress function of second order is obtained. It is equal to the sum of the background and non-conventional parts. The latter results in a continuation of the stresses within the core region, and the cut-off at the core's boundary is avoided. The asymptotic properties of the second order stresses are studied. New length scales of the "gauge" origin are provided, which could characterize an exterior structure of the dislocation core.

We do not discuss in detail a complicated theme such as the dislocation cores (see [3], [4], [9], [10], [32], and [33]). For instance, [34] and [35] are the first attempts to incorporate the lattice periodicity and to display the finiteness of the cores. Early attempts at treating the screw dislocations and their cores atomistically are given in [36], [37], and [38]. A singularity-less screw dislocation has also been obtained in [39] by means of the quasi-continuum approach (see [40] as well). In their turn, the gauge fields are important in modern condensed matter physics (see [41], [42], and [43]). Certain applications of [11] and [12] can

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[1]For a special choice of the parameters, the gauge Lagrangian in [16]–[19] is equivalent to the Lagrangians either in [14] or in [15]. Note that the most general eight-parameter three-dimensional geometric Lagrangian is known [31], which includes, in addition to the Hilbert–Einstein term, the terms quadratic in the components of the differential-geometric torsion and curvature.

be found in [44]– [49].

The paper consists of six sections. Section 1 is introductory (see also [14]– [19]). Section 2 outlines the Einstein-type gauge equation. Section 3 specifies the perturbative approach. The gauge equation is solved, and the modified stress potential is obtained in Section 4. The stress fields and their asymptotics are investigated in Section 5. Section 6 closes the paper. Details of the calculation are given in Appendices A and B. The present paper is a refined and improved (concerning the large distance behaviour of the stresses) version of [50]. Bold-faced letters are reserved for second-rank tensors, and appropriate indices can easily be restored.

2   The Einstein-type gauge equation

The Einsteinian gauge equation is outlined in the present section. For more on the appropriate differential geometry, one should refer to [10], [42], and [51]. The Eulerian picture is chosen in the present approach instead of the Lagrangian one accepted in [15]. The initial and final states of the dislocated body are referred to the coordinate systems $\{x^i\}$ and $\{x^a\}$, respectively. The corresponding squared length elements are expressed as $g_{ij}dx^i dx^j$ and $\eta_{ab}dx^a dx^b$ (throughout the paper, the indices repeated imply summation). Let us define the frame components e^a_i by the relation $\partial_i = e^a_i \partial_a$ (henceforth the partial derivatives $\partial/\partial x^i$ are denoted by ∂_i). The co-frame components $\mathcal{E}_a^i$ are given by the one-form $dx^i = \mathcal{E}_a^i dx^a$. The components $\mathcal{E}_a^i$ and their duals e^a_i are orthogonal: $e^a_i \mathcal{E}_b^i = \delta^a_b$, $e^a_i \mathcal{E}_a^j = \delta^j_i$. For the metric η_{ab} we get $\eta_{ab} = g_{ij} \mathcal{E}_a^i \mathcal{E}_b^j$.

The Eulerian strain tensor is referred to the deformed state, and it measures a deviation between the final and initial configurations [10]. Let us map an initial state to the deformed one: $\mathbf{x} \longmapsto \boldsymbol{\xi}(\mathbf{x})$. Then the difference

$$\eta_{ab}d\xi^a d\xi^b - g_{ij}dx^i dx^j = 2e_{ab}d\xi^a d\xi^b, \tag{2.1}$$

where

$$2e_{ab} \equiv \eta_{ab} - g_{ab}, \qquad g_{ab} \equiv g_{ij}\mathcal{B}_a^i \mathcal{B}_b^j, \tag{2.2}$$

defines the Eulerian strain tensor $(\mathbf{e})_{ab} \equiv e_{ab}$. The metric g_{ab} in (2.2) is called the Cauchy deformation tensor. Here $\mathcal{B}_a^i$ are given by the one-form $dx^i = \mathcal{B}_a^i d\xi^a$ as follows [10]:

$$\mathcal{B}_a^i \equiv \frac{\partial x^i}{\partial \xi^a} = \mathcal{E}_a^i - \mathcal{E}_b^i \overset{(\eta)}{\nabla}_a u^b, \tag{2.3}$$

provided that the displacement $\boldsymbol{\xi} - \mathbf{x}$ is expanded as $\xi^i - x^i = u^a \mathcal{E}_a^i$. The covariant derivative $\overset{(\eta)}{\nabla}_a$ in (2.3) is defined by the requirement that the components $\mathcal{E}_a^i$ are covariantly constant:

$$\overset{(\eta)}{\nabla}_a \mathcal{E}_b^i \equiv \partial_a \mathcal{E}_b^i - \left\{ \begin{matrix} c \\ ab \end{matrix} \right\}_\eta \mathcal{E}_c^i = 0, \tag{2.4}$$

where $\left\{ \begin{matrix} c \\ ab \end{matrix} \right\}_\eta$ is the Christoffel symbol of second kind. The metric $\eta_{ab} = \mathcal{E}_a^i \mathcal{E}_{bi}$ is also covariantly constant because of (2.4). In turn, (2.4) allows one to express the Christoffel symbols in terms of the metric η_{ab} (see [42]).

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To implement the gauging of the group $T(3)$, we extend the co-frame components $\mathcal{B}_a{}^i$ (2.3) by means of the so-called compensating fields:

$$\mathcal{B}_a{}^i \equiv \frac{\partial x^i}{\partial \xi^a} - \varphi_a{}^i = \mathcal{E}_a{}^i - \left(\mathcal{E}_b{}^i \overset{(\eta)}{\nabla}_a u^b + \varphi_a{}^i \right). \tag{2.5}$$

The entries $\varphi_a{}^i$ are the translational gauge potentials, which behave under the local transformations $x^i \longrightarrow x^i + \eta^i(x)$ as follows:

$$\begin{aligned}
\frac{\partial x^i}{\partial \xi^a} &\longrightarrow \frac{\partial x^j}{\partial \xi^a} \left(\delta^i_j + \frac{\partial \eta^i}{\partial x^j} \right), \\
\varphi_a{}^i &\longrightarrow \varphi_a{}^i + \frac{\partial x^j}{\partial \xi^a} \frac{\partial \eta^i}{\partial x^j}.
\end{aligned} \tag{2.6}$$

The shifts (2.6) ensure the gauge invariance of $\mathcal{B}_a{}^i$ (2.5) (and of the definitions (2.2), as well). Motivation of (2.5) should be traced back to $T(3) \otimes SO(3)$-gauging and to the corresponding Cartan structure equations [11] (see also [52] and [53]). The occurrence of the non-trivial core region for the screw dislocation in question (i.e., the appearance of the short-ranged stresses) should be associated with the gauge variables $\varphi_a{}^i$. The Eulerian strain (2.2) takes the gauged form:

$$2e_{ab} = \overset{(\eta)}{\nabla}_a u_b + \varphi_{ab} + \overset{(\eta)}{\nabla}_b u_a + \varphi_{ba} - \left(\overset{(\eta)}{\nabla}_a u_b + \varphi_{ab} \right) \left(\overset{(\eta)}{\nabla}_b u_a + \varphi_{ba} \right). \tag{2.7}$$

When φ is zero, (2.7) is reduced to the conventionally-looking (background) strain tensor in the Eulerian picture [10].

The differential-geometric approach of the present paper is the same as in [15], i.e., the so-called *teleparallel* framework (see [52] for a quick remind) is adopted as the most suitable for describing the dislocations [51]. Let us consider the Riemann–Christoffel curvature tensor $\mathrm{R}_{abc}{}^d$:

$$\mathrm{R}_{abc}{}^d = \partial_a \left\{ \begin{matrix} d \\ bc \end{matrix} \right\}_g - \partial_b \left\{ \begin{matrix} d \\ ac \end{matrix} \right\}_g + \left\{ \begin{matrix} d \\ ae \end{matrix} \right\}_g \left\{ \begin{matrix} e \\ bc \end{matrix} \right\}_g - \left\{ \begin{matrix} d \\ be \end{matrix} \right\}_g \left\{ \begin{matrix} e \\ ac \end{matrix} \right\}_g, \tag{2.8}$$

where the Christoffel symbols are calculated for the metric g_{ab} (2.2) (the subscript 'g') given by $\mathcal{B}_a{}^i$ (2.5). The metric g_{ab} is covariantly constant, i.e., $\overset{(g)}{\nabla}_a g_{bc} = 0$ is fulfilled, where $\overset{(g)}{\nabla}_a$ is defined similar to (2.4). We obtain from $\overset{(\eta)}{\nabla}_a \eta_{bc} = 0$ the following relation between the Christoffel symbols:

$$\left\{ \begin{matrix} c \\ ab \end{matrix} \right\}_\eta - \left\{ \begin{matrix} c \\ ab \end{matrix} \right\}_g = 2e_{ab}{}^c, \tag{2.9.1}$$

$$2e_{ab}{}^c \equiv g^{ce} \left(\overset{(\eta)}{\nabla}_a e_{be} + \overset{(\eta)}{\nabla}_b e_{ae} - \overset{(\eta)}{\nabla}_e e_{ab} \right). \tag{2.9.2}$$

where (2.2) is taken into account [10].

Let us define the Einstein tensor $G^{ef} \equiv \frac{1}{4} \mathcal{E}^{eab} \mathcal{E}^{fcd} \mathrm{R}_{abcd}$, where $\mathcal{E}^{abc}$ is the Levi–Civita tensor defined by means of the metric η_{ab}. Then, the Einstein-type gauge equation [15] takes the form

$$G^{ef} = \frac{1}{2\ell} \left(\sigma^{ef} - (\sigma_{\mathrm{bg}})^{ef} \right). \tag{2.10}$$

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Here ℓ is a constant factor at the Hilbert–Einstein gauge Lagrangian. The geometry of the deformed state is Euclidean in the Eulerian approach. The corresponding curvature $\overset{(\eta)}{\mathrm{R}}{}_{abc}{}^d$ is zero for the metric η_{ab}. We substitute (2.9.1) into (2.8) and use the vanishing of $\overset{(\eta)}{\mathrm{R}}{}_{abc}{}^d$. Then, (2.10) is re-expressed :

$$-\mathcal{E}^{eab}\mathcal{E}^{fcd}\,\overset{(\eta)}{\nabla}_a\,\overset{(\eta)}{\nabla}_c\,e_{bd} \;=\; \frac{1}{2\ell}\left(\sigma^{ef} - (\sigma_{\mathrm{bg}})^{ef}\right) + 2\mathcal{E}^{eab}\mathcal{E}^{fcd}e_{adl}\,e_{bc}{}^{l}. \tag{2.11}$$

The differential-geometric torsion, as an independent degree of freedom, is not considered. It is just the Riemann–Christoffel curvature that is subject to the gauge equation (2.10). Therefore, (2.11) governs only the variables related to the metric, i.e., the corresponding strains.

The variational derivation of (2.10) can be discussed along the line of [15]. The right-hand side of (2.10) is given by $(2\ell)^{-1}(\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\mathrm{bg}})$, where $\boldsymbol{\sigma}_{\mathrm{bg}}$ implies the background stress tensor. The deviation of the stress tensor of the model from $\boldsymbol{\sigma}_{\mathrm{bg}}$ plays the role of the driving source in the gauge equation. The parameter ℓ characterizes an energy scale intrinsic to the gauge field $\boldsymbol{\varphi}$: it makes the driving source dimensionless. In the present paper, $\boldsymbol{\sigma}_{\mathrm{bg}}$ implies the stress field of the straight screw dislocation lying along an infinite cylindric body. Both $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}_{\mathrm{bg}}$ respect the equilibrium equations:

$$\overset{(\eta)}{\nabla}_a\,\sigma^{ab} = 0, \qquad \overset{(\eta)}{\nabla}_a\,\left(\sigma_{\mathrm{bg}}\right)^{ab} = 0\,. \tag{2.12}$$

A more detailed consideration of the gauge geometry behind the model in question should be done elsewhere, but several refs. should be mentioned in addition to those listed in [15]. For instance, useful indications concerning the translational gauge geometry can be found in [54] and [55]. A topological picture is proposed in [56], which includes the dislocations and extra-matter by means of the torsion and non-metricity, respectively. Moreover, [57] provides a further development of the geometric approach [31].

3 Specification of the gauge equation

3.1 The stress function method

We shall investigate the gauge equation (2.11) using the method of stress functions proposed in [5] and [7] for solving the internal stress problems in the incompatible elasticity. An exposition of [7] can be found in ref. [10] devoted to a review of the dislocation problems in non-linear elasticity. Certain details omitted below can be restored with the help of [7] and [10].

We shall use the stress function approach in a successive approximation form. Let us represent the strain and the stress tensors perturbatively:

$$\mathbf{e} \approx \overset{(1)}{\mathbf{e}} + \overset{(2)}{\mathbf{e}}, \qquad \boldsymbol{\sigma} \approx \overset{(1)}{\boldsymbol{\sigma}} + \overset{(2)}{\boldsymbol{\sigma}}, \tag{3.1}$$

where $\overset{(2)}{\mathbf{e}}$ and $\overset{(2)}{\boldsymbol{\sigma}}$ are of second order smallness in comparison with $\overset{(1)}{\mathbf{e}}$ and $\overset{(1)}{\boldsymbol{\sigma}}$. The representation (2.7) implies that each contribution in (3.1) consists of two parts: owing to the background and to the non-conventional origin. Following [7], we shall investigate only the stress problem. Finding the relationship between the non-conventional stresses and the

gauge potentials is beyond the scope of the present paper. Substituting (3.1) into (2.11) and (2.12), we obtain equations of the first ($i = 1$) and second ($i = 2$) orders:

$$\boldsymbol{\nabla}\cdot \overset{(i)}{\boldsymbol{\sigma}}= 0\,,\tag{3.2.1}$$

$$\mathbf{Inc}\ \overset{(i)}{\mathbf{e}} = \frac{1}{2\ell}\,\boldsymbol{\delta}\,\overset{(i)}{\boldsymbol{\sigma}} + \overset{(i-1)}{\mathbf{Q}}\,.\tag{3.2.2}$$

The tensor notations [10] are used in (3.2). For instance, the left-hand side of (3.2.1) takes the form of the divergence of the tensor of second rank. The notation in (3.2.2) is:

$$\left(\mathbf{Inc}\ \overset{(i)}{\mathbf{e}}\right)^{ab} \equiv -\mathcal{E}^{acd}\mathcal{E}^{bfe}\nabla_c\nabla_f\,\overset{(i)}{e}_{de}\,,\tag{3.3.1}$$

$$\left(\boldsymbol{\delta}\,\overset{(i)}{\boldsymbol{\sigma}}\right)^{ab} \equiv \overset{(i)}{\sigma}{}^{ab} - \left(\overset{(i)}{\boldsymbol{\sigma}}_{\mathrm{bg}}\right)^{ab}\,,\tag{3.3.2}$$

$$\overset{(0)}{Q}{}^{ab} \equiv 0\,, \qquad \overset{(1)}{Q}{}^{ab} \equiv 2\,\mathcal{E}^{acd}\mathcal{E}^{bfe}\,\overset{(1)}{e}_{cel}\,\overset{(1)}{e}_{df}{}^{l}\,,\tag{3.3.3}$$

where '**Inc**' is the double curl *incompatibility operator*, $\boldsymbol{\nabla}$ is the covariant derivative $\overset{(\eta)}{\nabla}_a$ ($\equiv \nabla_a$), and the indices are raised and lowered by means of the metric $\boldsymbol{\eta}$.

Equations (3.2) look similar to the conventional equilibrium and incompatibility laws: see Eqs. (622) and (623) in [10]. The equilibrium equations of the first and second orders are given by (3.2.1). The gauge equations (3.2.2) play the role of non-conventional incompatibility conditions. However, there exists a distinction that is due to $(2\ell)^{-1}\boldsymbol{\delta}\,\overset{(i)}{\boldsymbol{\sigma}}$ in (3.2.2). This term is just responsible for the short-ranged behaviour of the gauge parts of the resulting stress functions. Moreover, $\overset{(1)}{\mathbf{Q}}$ in (3.3.3) is free from the torsion tensor in our approach.

The elastic energy of an isotropic body is chosen in the Eulerian representation as follows:

$$W(\mathbf{e}) = jI_1^2(\mathbf{e}) + kI_2(\mathbf{e}) + l'I_1^3(\mathbf{e}) + m'I_1(\mathbf{e})\,I_2(\mathbf{e}) + n'I_3(\mathbf{e})\,,\tag{3.4}$$

where $j = \mu + \lambda/2$ and $k = -2\mu$ are the elastic moduli of second order (λ and μ are the Lamé constants), and l', m', and n' are the elastic moduli of third order. Once $W(\mathbf{e})$ has been chosen in the form (3.4), the constitutive law relates $\overset{(i)}{\mathbf{e}}$ with $\overset{(i)}{\boldsymbol{\sigma}}$ ($i = 1, 2$) as follows [7]:

$$\overset{(i)}{\mathbf{e}} = C_1 I_1\!\left(\overset{(i)}{\boldsymbol{\sigma}}\right)\boldsymbol{\eta} + C_4\,\overset{(i)}{\boldsymbol{\sigma}} + \overset{(i-1)}{\boldsymbol{\Psi}}\,,\tag{3.5}$$

where $\overset{(0)}{\boldsymbol{\Psi}}\equiv 0$ and

$$\overset{(1)}{\boldsymbol{\Psi}} \equiv \left(C_2 I_1^2\!\left(\overset{(1)}{\boldsymbol{\sigma}}\right) + C_3 I_2\!\left(\overset{(1)}{\boldsymbol{\sigma}}\right)\right)\boldsymbol{\eta} + C_5 I_1\!\left(\overset{(1)}{\boldsymbol{\sigma}}\right)\overset{(1)}{\boldsymbol{\sigma}} + C_7 I_3\!\left(\overset{(1)}{\boldsymbol{\sigma}}\right)\left(\overset{(1)}{\boldsymbol{\sigma}}\right)^{-1}\,.\tag{3.6}$$

Here, the $I_{1,2,3}(\cdot)$ are the tensor invariants [58]. The numerical coefficients C_1 and C_4 are:

$$C_1 = -(2\mu)^{-1}\frac{\nu}{1+\nu}\,, \qquad C_4 = (2\mu)^{-1}\,,\tag{3.7}$$

where $\nu = \lambda/(2(\lambda + \mu))$ is the Poisson ratio. The coefficients C_2, C_3, C_5, and C_7 can be expressed (see [7] and [10]) in terms of the elastic moduli of second and third order (3.4),

although this is not used below. More details on the relation of λ, μ and l', m', n' with the elastic moduli of crystals can be found in [4] and [10].

The equilibrium equations (3.2.1) should be fulfilled with the help of the Kröner ansatz:

$$\overset{(i)}{\boldsymbol{\sigma}} = \mathbf{Inc}\ \overset{(i)}{\boldsymbol{\chi}}\,. \tag{3.8}$$

Substituting the constitutive relations (3.5) into (3.2.2) and using (3.8), we obtain equations for the components of the stress potential $\overset{(i)}{\boldsymbol{\chi}}$:

$$\Delta\Delta\ \overset{(i)}{\chi}_{ab} + a\Big(\nabla_a\nabla_b - \eta_{ab}\Delta\Big)\Delta I_1\big(\overset{(i)}{\chi}\big) + \Big((1-a)\nabla_a\nabla_b + a\,\eta_{ab}\Delta\Big)\nabla^c\nabla^d\ \overset{(i)}{\chi}_{cd} -$$
$$- \Delta\Big(\nabla_a\nabla_c\ \overset{(i)}{\chi}{}^c{}_b + \nabla_b\nabla_c\ \overset{(i)}{\chi}{}^c{}_a\Big) = \kappa^2\big(\boldsymbol{\delta}\,\overset{(i)}{\boldsymbol{\sigma}}\big)_{ab} + 2\mu\ \overset{(i)}{S}{}_{(ab)}\,, \tag{3.9}$$

where

$$\overset{(1)}{S}{}_{ab} \equiv 0\,, \qquad \overset{(2)}{S}{}_{(ab)} \equiv \overset{(1)}{Q}{}_{(ab)} - \Big(\mathbf{Inc}\ \overset{(1)}{\boldsymbol{\Psi}}\Big)_{(ab)}\,,$$

Δ is the Laplacian, and the $\boldsymbol{\delta}\,\overset{(i)}{\boldsymbol{\sigma}}$ are expressed by means of (3.3.2) and (3.8). In addition, $\overset{(1)}{Q}$ and $\overset{(1)}{\boldsymbol{\Psi}}$ are given by (3.3.3) and (3.6), accordingly. The curly brackets around the indices imply symmetrization, and we use the dimensionless parameters $\kappa^2 \equiv \mu/\ell$ and a (see [11] and [12]):

$$a \equiv \frac{\lambda}{3\lambda + 2\mu} = \frac{1}{1+\nu^{-1}}\,, \qquad 1 - a = \frac{2(\lambda+\mu)}{3\lambda + 2\mu} = \frac{1}{1+\nu}\,. \tag{3.10}$$

3.2   The gauge equations in the first and second orders

Let us adjust (3.9) to the special problem in question. We replace the derivatives ∇_a by the partial derivatives ∂_a, where x^a are the coordinates in the final state, and assume $\partial_3 \equiv 0$ (see [7] and [10]). Conventional notation is adopted for the components of the stress potential which are non-trivial [51]:

$$\mu\ \overset{(i)}{\phi} \equiv \partial_2\ \overset{(i)}{\chi}_{13} - \partial_1\ \overset{(i)}{\chi}_{23}\,, \qquad\qquad i = 1,\,2\,,$$
$$f \equiv \overset{(2)}{\chi}_{33}\,, \quad p \equiv -\partial_{11}^2\ \overset{(2)}{\chi}_{22} - \partial_{22}^2\ \overset{(2)}{\chi}_{11} + 2\,\partial_{12}^2\ \overset{(2)}{\chi}_{12}\,. \tag{3.11}$$

The other components of $\overset{(i)}{\boldsymbol{\chi}}$ are zero. The background stress tensor $\boldsymbol{\sigma}_{\mathrm{bg}}$ is also given by (3.8), but the corresponding stress potential is labelled appropriately: $\overset{(i)}{\boldsymbol{\chi}}_{\mathrm{bg}}$.

3.2.1   The first order

In the first order, only the stress potential $\overset{(1)}{\phi}$ (3.11) is non-zero for the screw dislocation. The corresponding governing equation appears from (3.9) as follows [15]:

$$(\Delta - \kappa^2)\big(\overset{(1)}{\phi} - \overset{(1)}{\phi}_{\mathrm{bg}}\big) = b\,\delta^{(2)}(x)\,, \tag{3.12}$$

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where $\overset{(1)}{\phi}_{\text{bg}} \equiv (-b/2\pi) \log \rho$ is the background stress potential, and b is the Burgers vector length. The Burgers vector is parallel to the line of the screw dislocation, and its length is the perturbative expansion parameter. The axial symmetry of the final state stimulates the usage of the cylindric coordinates ρ, φ, and z instead of $\{x^a\}$ (ρ and φ are chosen in the (x^1, x^2)-plane and $z \equiv x_3$). We obtain from (3.12) the stress potential of the first order:

$$\overset{(1)}{\phi} = \overset{(1)}{\phi}_{\text{bg}} - f_S, \qquad f_S \equiv (b/2\pi) K_0(\kappa\rho), \tag{3.13}$$

where K_0 is the modified Bessel function [59].

The stress $\sigma_{\phi z}$ is non-trivial for the modified screw dislocation in the first order, and we express it, using (3.8) and (3.11):

$$\sigma_{\phi z} = -\mu \, \partial_\rho \overset{(1)}{\phi} = \frac{b\mu}{2\pi} \rho^{-1} \left(1 - \kappa\rho K_1(\kappa\rho)\right). \tag{3.14}$$

Equation (3.14) demonstrates a core region at $\rho \lesssim \kappa^{-1}$: the gauge correction to the classical long-ranged law $1/\rho$ is exponentially small outside this region. Inside it, the law $1/\rho$ is replaced by another non-singular one. More detailed information on the numerical behaviour of (3.14) (including a treatment of κ^{-1} in terms of interatomic spacing) can be found in [14] and [17]. In the present paper, it is assumed that $b = O(\kappa^{-1})$. Solution (3.14) is in agreement with [14], [17] (the translational gauging), [20] (the non-local elasticity) and [22], [26], and [27] (the strain gradient elasticity). This is because the Helmholtz-type governing equations similar to (3.12) are essential in the approaches mentioned.

Certain analogies in the structure of the tensor laws governing the electrostatic of dielectrics and the elastostatic problems have been discussed in [60]. It looks hopeful that the short-ranged constituent of the first order solution presented here is also falling into the class of problems considered in [60]. In addition, within an independent framework though, strongly localized stress potentials turn out to be also responsible for the Debye-like screening effects in the dislocation arrangements [61].

3.2.2 The second order

In the second order, from (3.9) we obtain the following gauge equations [2]:

$$-\partial_{22}^2 \left[(1-a)p + a\Delta f - \kappa^2(f - f_{\text{bg}})\right] = 2\mu \left[Q_{11} + \partial_{22}^2 \Psi_{33}\right],$$

$$-\partial_{11}^2 \left[(1-a)p + a\Delta f - \kappa^2(f - f_{\text{bg}})\right] = 2\mu \left[Q_{22} + \partial_{11}^2 \Psi_{33}\right], \tag{3.15.1}$$

$$\partial_{12}^2 \left[(1-a)p + a\Delta f - \kappa^2(f - f_{\text{bg}})\right] = -2\mu \, \partial_{12}^2 \Psi_{33},$$

$$(1-a)\Delta\Delta f + a\Delta p - \kappa^2(p - p_{\text{bg}})$$

$$= 2\mu \left[Q_{33} - \partial_{12}^2\left(\Psi_{12} + \Psi_{21}\right) + \partial_{11}^2 \Psi_{22} + \partial_{22}^2 \Psi_{11}\right]. \tag{3.15.2}$$

Equations (3.15) describe the stress potentials of second order f and p (3.11). In addition, there are equations to determine $\overset{(2)}{\phi}$. But since $\overset{(2)}{\phi}_{\text{bg}}$ is zero [7], we put consistently $\overset{(2)}{\phi} \equiv 0$.

---

[2]Henceforth, $\mathbf{Q}$ and $\mathbf{\Psi}$ are used without the superscript.

Further, it is necessary to express $\mathbf{Q}$ in (3.3.3) and $\boldsymbol{\Psi}$ in (3.6) in terms of the first order solution (3.13). Taking $\partial_3 = 0$ into account and using $e_{ab}{}^c$ (2.9.2), we obtain the following non-zero components:

$$Q_{11} = Q_{22} = \frac{\left(\Delta \overset{(1)}{\phi}\right)^2}{4}, \tag{3.16.1}$$

$$Q_{33} = \left(\partial_{12}^2 \overset{(1)}{\phi}\right)^2 - \partial_{11}^2 \overset{(1)}{\phi}\, \partial_{22}^2 \overset{(1)}{\phi} + \frac{\left(\Delta \overset{(1)}{\phi}\right)^2}{4}. \tag{3.16.2}$$

In turn, the corresponding components of $\boldsymbol{\Psi}$ are expressed standardly (see [7] and [10]). Using (3.16.2), we obtain the combination that we are interested in:

$$Q_{33} - 2\partial_{12}^2 \Psi_{12} + \partial_{11}^2 \Psi_{22} + \partial_{22}^2 \Psi_{11}$$

$$\tag{3.17}$$

$$= \Delta \Psi_{33} + \left(1 - 2\mu^2 C_7\right) \Phi + \frac{\left(\Delta \overset{(1)}{\phi}\right)^2}{4},$$

where

$$\Psi_{33} \equiv -\mu^2 C_3 \left(\left(\partial_1 \overset{(1)}{\phi}\right)^2 + \left(\partial_2 \overset{(1)}{\phi}\right)^2 \right),$$

$$\tag{3.18}$$

$$\Phi \equiv \left(\partial_{12}^2 \overset{(1)}{\phi}\right)^2 - \partial_{11}^2 \overset{(1)}{\phi}\, \partial_{22}^2 \overset{(1)}{\phi}.$$

Equations (3.16) and (3.17) look unconventionally owing to the presence of $(\Delta \overset{(1)}{\phi})^2/4$. It is just the dependence of $\mathbf{Q}$ on the torsion that results in the absence of the contribution $(\Delta \overset{(1)}{\phi})^2/4$ in the components Q_{11}, Q_{22}, and Q_{33} obtained in [7]. Recall that the conventional incompatibility law requires the vanishing of the Einstein tensor calculated by means of the Riemann–Cartan curvature [51]. This latter includes (see [42]), in addition to the Riemann–Christoffel part (2.8), a contribution owing to the torsion tensor. The latter is identified as the dislocation density. That is, the dislocation density contributes into the driving source of the incompatibility law. On the contrary, according to [14], [15], and [17], a stress field owing to the background defect is chosen first. Since the torsion is not considered as an independent variable, Q_{11}, Q_{22}, and Q_{33} acquire the form (3.16).

Equations (3.15) allow for a correct limit to their classical version, which is respected by the background stress potentials of second order f_{bg} and p_{bg}. Let us pass to the classically-looking Q_{11}, Q_{22}, and Q_{12}:

$$Q_{11} = \partial_{22}^2 Q', \quad Q_{22} = \partial_{11}^2 Q', \quad Q_{12} = -\partial_{12}^2 Q'. \tag{3.19}$$

A specific value of the constant Q' arises from the requirement that $\overset{(2)}{\sigma}_{33}$ averaged over the cylinder's cross-section is zero (see [7] and [10]). Then, the equations that govern f_{bg} and p_{bg} take in our notation the form ($\kappa \to 0$)

$$\Delta\Delta f_{\mathrm{bg}} = k \left[\Delta(\Psi_{33}^{\mathrm{bg}} + Q') + (1 - a)(1 - 2\mu^2 C_7)\,\Phi_{\mathrm{bg}} \right],$$

$$\tag{3.20}$$

$$(1 - a)\, p_{\mathrm{bg}} + a\,\Delta f_{\mathrm{bg}} = -2\mu \left(\Psi_{33}^{\mathrm{bg}} + Q' \right),$$

where

$$k \equiv \frac{2\mu}{1 - 2a} = 2\mu \frac{1 + \nu}{1 - \nu}. \tag{3.21}$$

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Moreover, Ψ_{33}^{bg} and Φ_{bg} are given by (3.18), provided that $\overset{(1)}{\phi}$ is replaced by $\overset{(1)}{\phi}_{\mathrm{bg}}$.

Let us turn to (3.16). In the present approach, $\left(\Delta \overset{(1)}{\phi}\right)^2$ is the square of the density distribution of the modified screw dislocation (see [14], [15], and [17]):

$$\left(\Delta \overset{(1)}{\phi}\right)^2 = \left(\frac{b}{2\pi}\kappa^2 K_0(\kappa\rho)\right)^2 .\tag{3.22}$$

For large distances, $K_0(\kappa\rho)$ decays exponentially, and $\left(\Delta \overset{(1)}{\phi}\right)^2$ given by (3.22) can approximately be replaced by zero. Therefore, the components (3.16) take, also approximately, their conventional form. Then, three equations (3.15.1) reduce to a single one. However, $\Delta \overset{(1)}{\phi}$ is not negligible for sufficiently moderate $\kappa\rho$, and some care inside the core region $\rho \lesssim \kappa^{-1}$ is required. In other words, this might be an indication for extension of the geometric framework by means of the differential-geometric torsion. But this would, in turn, imply that the teleparallel description is abandoned.

Instead, we shall establish an "effective" picture, which should be viewed as still contained within the teleparallel framework. However, this description is expected to incorporate certain features of the approach extended differential-geometrically. Indeed, an independent non-trivial contribution owing to the torsion would lead to the following equation, instead of (3.12):

$$\Delta \overset{(1)}{\phi}_{\mathcal{T}} = \kappa^2\left(\overset{(1)}{\phi}_{\mathcal{T}} - \overset{(1)}{\phi}_{\mathrm{bg}}\right) + \mathcal{T}.\tag{3.23}$$

Here $\mathcal{T}$ is a suitable density caused by the non-triviality of the torsion components, say, $T_{12}^3 = -T_{21}^3$ (this is just appropriate for the screw dislocation along Oz, [51]). The notation $\overset{(1)}{\phi}_{\mathcal{T}}$ implies the corresponding solution at a given $\mathcal{T}$. Being considered as an additional source of incompatibility, $\mathcal{T}$ can be assigned to possess near Oz a series expansion with arbitrary, though adjustable, coefficients. As a result, $\overset{(1)}{\phi}_{\mathcal{T}}$ can also acquire, in comparison with $\overset{(1)}{\phi}$ (3.13), certain modifications near $\rho = 0$.

Therefore, $\left(\Delta \overset{(1)}{\phi}\right)^2$ is replaced, on an extended treatment, by $\left(\Delta \overset{(1)}{\phi}_{\mathcal{T}}\right)^2$. This can be effectively accounted for in the present framework as well. Let us introduce a piece-wisely constant density to "regularize" $\left(\Delta \overset{(1)}{\phi}\right)^2$ as follows [50]:

$$\left(\Delta \overset{(1)}{\phi}\right)^2 \sim \left(\frac{b}{\pi\rho_*^2}\right)^2 h_{[0,\,\rho_*]}(\rho),\tag{3.24}$$

where $h_{[0,\,\rho_*]}(\rho)$ is unity for $\rho \in [0, \rho_*]$ (i.e., within a disc) or zero otherwise. It is crucial that (3.24) should not be treated as a replacement to be iteratively improved. Let us use (3.24) in (3.16.1). Then, an analogue of (3.19) is valid, where the corresponding "potential" $\widetilde{g}$ is present:

$$\widetilde{g} = \frac{b^2}{8\pi^2\rho_*^2}\left(\frac{\rho^2}{\rho_*^2} - 1\right)h_{[0,\,\rho_*]}(\rho) + \mathcal{C}.\tag{3.25}$$

The constants $\mathcal{C}$ and ρ_* should be specified later. Both $\dfrac{b}{2\pi}\kappa^2 K_0(\kappa\rho)$ and $\dfrac{b}{\pi\rho_*^2}h_{[0,\,\rho_*]}(\rho)$ are δ-like for κ and $1/\rho_*$ large enough, respectively. Considered as the surface densities, they

are properly normalized. Therefore, the replacement (3.24) looks better, provided that its δ-like character is sharper.

Using (3.19), where $\widetilde{g}$ given by (3.25) is substituted, from (3.15) we obtain the following equations [50]:

$$\left(\Delta - \kappa^2\right)\left(\Delta + \frac{\kappa^2}{1 - 2a}\right)(f - f_{\text{bg}}) = k\,\mathcal{R}\,, \tag{3.26.1}$$

$$p = -\frac{a}{1 - a}\,\Delta f - \frac{2\mu}{1 - a}\left(\Psi_{33} + \widetilde{g}\right) + \frac{\kappa^2}{1 - a}\left(f - f_{\text{bg}}\right). \tag{3.26.2}$$

Here, f_{bg} respects the first equation (3.20), and k is given by (3.21). The driving source in (3.26.1) is defined as follows:

$$
\begin{aligned}
\mathcal{R} \;\equiv\; & \left(\Delta - \kappa^2\right)\!\left(\Psi_{33} + \widetilde{g} - \Psi_{33}^{\text{bg}} - Q'\right) \\[4pt]
+ \;\; & (1 - a)\left(1 - 2\mu^2 C_7\right)\!\left(\Phi - \Phi_{\text{bg}}\right) - \frac{1 - a}{4}\big(\Delta\,\overset{(1)}{\phi}\big)^2.
\end{aligned}
\tag{3.27}
$$

It is assumed that Ψ_{33} and Φ (or, analogously, Ψ_{33}^{bg} and Φ_{bg}) in (3.27) are given by (3.18) where $\overset{(1)}{\phi}$ (or, correspondingly, $\overset{(1)}{\phi}_{\text{bg}}$) is substituted appropriately. In addition, $\big(\Delta\,\overset{(1)}{\phi}\big)^2$ is kept in (3.27) only formally, as a symbol. The first equation in (3.26.1) (would be called, after [29] and [30], the non-homogeneous *bi-Helmholtz equation* [3]) is just to be solved in what follows to determine the stress function f. Equation (3.26.2) is needed only to express the stress component $\sigma_{zz} = p$.

The governing equations (3.26) are essentially similar to equations that should be expected under a consideration extended by means of the torsion (see also explanations in Section 5.3). The actual derivation of (3.26) incorporates (3.16) and (3.17), which are subject to (3.24). Therefore, the teleparallel framework is valid only approximately. However, the free parameter ρ_* is coming to play by means of (3.24), and this supports the similarity noted. Indeed, the arbitrariness owing to ρ_* is reminiscent of a freedom caused by the non-triviality of appropriate torsion. Technical complexities, which might appear in the description based on (3.23), should be avoided now, since they deserve separate studying. Therefore, the strategy based on (3.24) looks appropriate. Equations (3.26) lead eventually to a self-consistent stress distribution without an artificial cut-off at the core.

3.3   The driving source of the gauge equation

Before solving (3.26.1), simplifications for $\mathcal{R}$ given by (3.27) are in order. It is convenient to investigate $\mathcal{R}$ multiplied by ρ^2. We use (3.13) and (3.18) and keep the same notation $\mathcal{R}$ after the multiplication. After re-scaling the radial coordinate $\kappa\rho \mapsto s$, we obtain approximately (see [50]):

$$\mathcal{R} \approx s^2 w(s) + \sum_{a=1}^{3} \mathcal{R}_a\,, \tag{3.28}$$

---

[3] See [29] and [30] for appropriate refs. and more examples of non-homogeneous bi-Helmholtz equations. A δ-driven differential equation analogous to (3.26.1) has already appeared in [15] as well.

where

$$X^{-2}\mathcal{R}_1 = \left(\tilde{c} + cs^2\right) K_1(s) \left(K_1(s) - \frac{2}{s}\right),$$

$$X^{-2}\mathcal{R}_2 \approx -\tilde{c}sK_1(s)\Delta_s\widetilde{\phi} \sim \frac{2\tilde{c}}{s_*^2} sK_1(s)\widetilde{h}_{[0,\,s_*]}(s), \qquad (3.29)$$

$$X^{-2}\mathcal{R}_3 \approx -2c\,s^2 K_1(s)\frac{d}{ds}\left(\Delta_s\widetilde{\phi}\right) = -2c\left(sK_1(s)\right)^2.$$

The following notation is accepted in (3.28) and (3.29):

$$\tilde{c} \equiv (1-a)(1-2\mu^2 C_7) - 4c, \qquad c \equiv \mu^2 C_3,$$

$$s^2\,w(s) \equiv X^2\,\frac{s^2}{s_*^4}\left[(1+a) - \frac{1}{2}\left(s^2 - s_*^2\right)\right]\widetilde{h}_{[0,\,s_*]}(s), \qquad (3.30)$$

where a and $1-a$ are given by (3.10), $s_* \equiv \kappa\rho_*$, and $\widetilde{h}_{[0,\,s_*]}(s)$ is unity at $s \in [0,\,s_*]$ or zero otherwise (we use $\mathcal{C} = Q'$ in (3.25)). Further, $\widetilde{\phi}$ in (3.29) implies $\overset{(1)}{\phi}$ with removed multiple $\frac{b}{2\pi}$. The factor $X^2 \equiv \left(\frac{b\,\kappa}{2\pi}\right)^2$ just points out the fact that the driving source is quadratic in b. Moreover, Δ_s is $s^{-1}\frac{d}{ds}\left(s\frac{d}{ds}\right)$, and K_0 and K_1 are the modified Bessel functions [59].

The following comments on (3.28) and (3.29) are in order. Classically, $\Delta\overset{(1)}{\phi}_{\mathrm{bg}}$ is the Dirac's delta-function, and its square would occur instead of (3.22). The equation for the corresponding stress function f_{bg} is conventionally considered for strictly positive ρ. Then, the corresponding driving source is not influenced by $\Delta\overset{(1)}{\phi}_{\mathrm{bg}}$. Therefore, it seems inappropriate to account for, at the same footing with (3.24), the contributions expressible in $\mathcal{R}$ by the differences $\Delta\overset{(1)}{\phi} - \Delta\overset{(1)}{\phi}_{\mathrm{bg}}$ or $\partial_\rho(\Delta\overset{(1)}{\phi} - \Delta\overset{(1)}{\phi}_{\mathrm{bg}})$. To put it differently, the regularization allowed classically "persists" into the non-conventional approach, and (3.28) and (3.29) take their actual form.

The asymptotic properties of $\mathcal{R}$ (3.28) are as follows. First, $\mathcal{R}$ is well localized since it contains the modified Bessel functions. At small s, we expand

$$\mathcal{R}(s) \simeq p_1\,s^{-2} + p_2\,\log s + p_3$$
$$+ \; s^2\left(p_4\,\log^2 s + p_5\,\log s + p_6\right) + o(s^2), \qquad (3.31)$$

where the numerical coefficients $p_1, p_2, \ldots, p_6$ are

$$p_1 = -X^2\,\tilde{c}, \qquad\qquad p_2 = 0,$$

$$p_3 = X^2\left(\frac{2\tilde{c}}{s_*^2} - \alpha c\right), \qquad p_4 = X^2\,\frac{\tilde{c}}{4},$$

$$p_5 = X^2\left(\frac{\tilde{c}}{s_*^2} - \frac{\tilde{c}}{4}\left(1 - 2\log\frac{\gamma}{2}\right) + (1-\alpha)\,c\right), \qquad (3.32)$$

$$p_6 = w(0) + X^2\left(1 - 2\log\frac{\gamma}{2}\right)\left(\left(1 - 2\log\frac{\gamma}{2} - \frac{8}{s_*^2}\right)\frac{\tilde{c}}{16} + (\alpha - 1)\frac{c}{2}\right),$$

with $\alpha = 1$ or $\alpha = 3$ in p_3, p_5, and p_6. Indeed, the calculation of $\mathcal{R}_3$ requires, as soon as (3.24) is imposed, the differentiation of the step-function. This would result in singularities in the

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driving source. Our regularized scheme can thus be destroyed. We use p_3, p_5, and p_6 with $\alpha = 1$, when $\mathcal{R}_3$ is simply omitted to express the neglect of the corresponding differentiation. Otherwise (for comparison), $\alpha = 3$ when $\mathcal{R}_3$ is calculated according to (3.29). However, α is left unspecified to give an indication of both possibilities. Moreover, in spite of $p_2 \equiv 0$, it is instructive to keep the corresponding term in (3.31). It is to be equated to zero at the end.

4   Solution of the gauge equation

We are going to solve (3.26.1) in two steps [50]. First, we consider the non-homogeneous Bessel equation

$$\left[s^2 \frac{d^2}{ds^2} + s\frac{d}{ds} - s^2 \right] G(s) = \mathcal{R}(s). \tag{4.1}$$

The method of variation of parameters [62] provides a general solution to (4.1). We choose the modified Bessel functions I_0 and K_0 [59] as two linearly independent solutions of the associated homogeneous Bessel equation. Solution to (4.1) appears as follows:

$$
\begin{aligned}
G(s) \;=\; \lim_{\epsilon \to 0} \Bigg[& I_0(s) \left(A(\epsilon) + \int_\epsilon^s K_0(t)\mathcal{R}(t)\,\frac{dt}{t} \right) \\
+ \;& K_0(s) \left(B(\epsilon) - \int_\epsilon^s I_0(t)\mathcal{R}(t)\,\frac{dt}{t} \right) \Bigg],
\end{aligned}
\tag{4.2.1}
$$

where

$$
\begin{aligned}
A(\epsilon) &\equiv - \int_\epsilon^\infty K_0(t)\mathcal{R}(t)\,\frac{dt}{t}, \\
B(\epsilon) &\equiv \text{const} + \int_\epsilon^1 \left(\frac{p_1}{t^3} + \frac{p_2}{t}\log t + \left(\frac{p_1}{4} + p_3 \right)\frac{1}{t} \right) dt.
\end{aligned}
\tag{4.2.2}
$$

The behaviour of $t^{-1}I_0(t)\mathcal{R}(t)$ and $t^{-1}K_0(t)\mathcal{R}(t)$ for small or large t is important for justification of (4.2). When t is small, the regularization in $G(s)$ is ensured by means of the specially constructed $A(\epsilon)$ and $B(\epsilon)$ from (4.2.2) (see Appendix A). When t is large, $K_0(t)\mathcal{R}(t)$ decays as e^{-2t}, whereas $I_0(t)\mathcal{R}(t)$ behaves, mainly, as a constant. Therefore, the infinity as an upper bound in $A(\epsilon)$ given by (4.2.2) is appropriate. The choice of the integration bounds implies that $G(s)$ decays exponentially for large s. The important arbitrariness in $B(\epsilon)$ from (4.2.2) should be stressed, which is due to the additive constant denoted as *const*.

Using Appendix A, it is straightforward to expand $G(s)$ for small s:

$$G(s) \simeq q_1\, s^{-2} + \sum_{i=0}^{3} q_{5-i} \log^i s + s^2 \sum_{i=0}^{3} q_{9-i} \log^i s + \dots. \tag{4.3}$$

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The numerical coefficients in (4.3) are expressed in terms of the parameters (3.32) as follows:

$$q_1 = \frac{p_1}{4}, \qquad q_2 = \frac{p_2}{6}, \qquad q_3 = \frac{p_1}{8} + \frac{p_3}{2},$$

$$q_4 = -\text{const} + \frac{3p_1}{4}, \qquad q_5 = -\text{const} \times \log\frac{\gamma}{2} - \mathcal{I}_K - \frac{p_1}{16}, \qquad (4.4)$$

$$q_6 = \frac{p_2}{24}, \qquad q_7 = \frac{p_1}{32} + \frac{p_3 - p_2}{8} + \frac{p_4}{4},$$

where $\mathcal{I}_K$ is given by (A8) in Appendix A, and *const* in q_4 and q_5 is introduced by (4.2.2). The coefficients q_8 and q_9 in (4.3) are practically too complicated and are not of importance below.

As a second step, we express the difference $f - f_{\text{bg}} \equiv k\,\mathcal{F}$, where $\mathcal{F}$ respects the non-homogeneous Bessel equation

$$\left[s^2\frac{d^2}{ds^2} + s\frac{d}{ds} + s^2\right]\mathcal{F}\left(\frac{s}{\mathcal{N}}\right) = \frac{s^2}{\mathcal{N}^2}G\left(\frac{\kappa}{\mathcal{N}}s\right). \qquad (4.5)$$

The modified stress potential of the second order appears as $f = f_{\text{bg}} + k\,\mathcal{F}$. For convenience, (4.5) is also written in terms of the new variable s, which is however defined differently: $s \equiv \mathcal{N}\rho$, where $\mathcal{N}^2 \equiv \dfrac{\kappa^2}{1 - 2a}$. We choose Y_0 and J_0 as the fundamental solutions of the homogeneous Bessel equation associated with (4.5) and obtain

$$\mathcal{F}(\rho) = C\,\widetilde{Y}_0(\mathcal{N}\rho) + D\,J_0(\mathcal{N}\rho) + I_{\mathcal{F}}(\rho),$$

$$I_{\mathcal{F}}(\rho) \equiv J_0(\mathcal{N}\rho)\int_\rho^\infty \widetilde{Y}_0(\mathcal{N}t)G(\kappa t)\,t\,dt - \widetilde{Y}_0(\mathcal{N}\rho)\int_\rho^\infty J_0(\mathcal{N}t)G(\kappa t)\,t\,dt, \qquad (4.6)$$

where $G(\cdot)$ is given by (4.2), and $\widetilde{Y}_0(s) \equiv (\pi/2)Y_0(s)$. Here the integrals are convergent at their upper bounds.

In the preceding consideration (see [50]), the choice of $C \neq 0$ and $D = 0$ has been made in $\mathcal{F}(\rho)$ from (4.6). However, in this case the stress field looks non-conventional for sufficiently large distances. In the present paper, we put C and D equal to zero, and thus $\mathcal{F}(\rho) = I_{\mathcal{F}}(\rho)$. The integral $I_{\mathcal{F}}(\rho)$ decays exponentially for large ρ, while for small $\mathcal{N}\rho$ we obtain (Appendix B)

$$\mathcal{F}(\rho) \simeq r_0 + r_1\log\rho + r_2\log^2\rho + \rho^2\sum_{i=0}^{3}r_{6-i}\log^i\rho + r_7\,\rho^4\log^3\rho + \ldots, \qquad (4.7)$$

where

$$r_0 = -\widetilde{\mathcal{I}}_Y + \log\left(\frac{\gamma}{2}\mathcal{N}\right)\widetilde{\mathcal{I}}_J, \qquad r_1 = \widetilde{\mathcal{I}}_J, \qquad r_2 = \frac{p_1}{8\kappa^2},$$

$$r_3 = \frac{p_2}{24}, \qquad r_4 = \left(1 - \frac{\mathcal{N}^2}{\kappa^2}\right)\frac{p_1}{32} - (1 - \log\kappa)\frac{p_2}{8} + \frac{p_3}{8}, \qquad (4.8)$$

$$r_7 = (\kappa^2 - \mathcal{N}^2)\frac{p_2}{384},$$

and p_1, p_2, and p_3 are given by (3.32). The coefficients r_5 and r_6 are given by (B6)–(B11), and $\widetilde{\mathcal{I}}_Y$ and $\widetilde{\mathcal{I}}_J$ are defined by (B10) in Appendix B.

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5 The stress tensor

5.1 The components $\sigma_{\rho\rho}$ and $\sigma_{\phi\phi}$

Therefore the modified stress potential of second order f takes the form

$$f = f_{\text{bg}} + kI_{\mathcal{F}}, \tag{5.1.1}$$

$$f_{\text{bg}} = -\widetilde{n} \log^2 \rho + d_1 \rho^2 + d_2 \log \rho, \qquad \widetilde{n} \equiv k \frac{p_1}{8\kappa^2}, \tag{5.1.2}$$

where $I_{\mathcal{F}}$ is given by (4.6), and the stress potential f_{bg} is in full agreement with [7]. The potential f_{bg} respects the following equation, which results from (3.20) for $\rho \neq 0$:

$$\Delta\Delta f_{\text{bg}} = \frac{-8\widetilde{n}}{\rho^4}. \tag{5.2}$$

Taking into account (3.8) and (3.11), we represent the stress tensor of the second order in the cylindrical coordinates as follows:

$$\overset{(2)}{\sigma}_{\rho\rho} = -\frac{1}{\rho}\frac{d}{d\rho}f, \qquad \overset{(2)}{\sigma}_{\phi\phi} = -\frac{d^2}{d\rho^2}f, \qquad \overset{(2)}{\sigma}_{zz} = p, \tag{5.3}$$

where f from (5.1) and p from (3.26.2) are substituted. The other components of $\overset{(2)}{\sigma}$ are zero. In the classical problem, we use (5.3) with f_{bg} from (5.1.2) and obtain

$$
\begin{aligned}
(\overset{(2)}{\sigma}_{\text{bg}})_{\rho\rho} &= 2\widetilde{n}\frac{\log\rho}{\rho^2} - \frac{d_2}{\rho^2} - 2d_1, \\
(\overset{(2)}{\sigma}_{\text{bg}})_{\phi\phi} &= -2\widetilde{n}\frac{\log\rho}{\rho^2} + \frac{2\widetilde{n} + d_2}{\rho^2} - 2d_1.
\end{aligned}
\tag{5.4}
$$

The free parameters d_1 and d_2 in (5.4) are given by the vanishing of $(\overset{(2)}{\sigma}_{\text{bg}})_{\rho\rho}$ on the boundaries of the hollow cylinder, e.g., $\rho = \rho_{\text{c}}$ and $\rho = \rho_{\text{e}} > \rho_{\text{c}}$:

$$\left.(\overset{(2)}{\sigma}_{\text{bg}})_{\rho\rho}\right|_{\rho=\rho_{\text{e}}} = \left.(\overset{(2)}{\sigma}_{\text{bg}})_{\rho\rho}\right|_{\rho=\rho_{\text{c}}} = 0. \tag{5.5}$$

Substitution of (5.4) into (5.5) allows us to define d_1 and d_2. For our purposes, it is more appropriate to assume that ρ_{e} is essentially greater than ρ_{c} (ρ_{e}/ρ is moderate). We approximately obtain

$$d_1 \approx \frac{\widetilde{n}}{\rho_{\text{e}}^2}\log\frac{\rho_{\text{e}}}{\rho_{\text{c}}}, \qquad d_2 \approx 2\widetilde{n}\log\rho_{\text{c}}, \tag{5.6}$$

and

$$
\begin{aligned}
(\overset{(2)}{\sigma}_{\text{bg}})_{\rho\rho} &\approx \frac{2\widetilde{n}}{\rho^2}\left(\log\frac{\rho}{\rho_{\text{c}}} - \left(\frac{\rho}{\rho_{\text{e}}}\right)^2\log\frac{\rho_{\text{e}}}{\rho_{\text{c}}}\right), \\
(\overset{(2)}{\sigma}_{\text{bg}})_{\phi\phi} &\approx \frac{2\widetilde{n}}{\rho^2}\left(1 - \log\frac{\rho}{\rho_{\text{c}}} - \left(\frac{\rho}{\rho_{\text{e}}}\right)^2\log\frac{\rho_{\text{e}}}{\rho_{\text{c}}}\right).
\end{aligned}
\tag{5.7}
$$

Note that $\widetilde{n}$ is proportional to b^2, and f_{bg} from (5.1.2) is indeed of second order in b. From (3.29), (4.2), and (4.6) it is seen that $I_{\mathcal{F}}$ is also quadratic in b.

Let us turn to the stress components (5.3) with f substituted from (5.1). The solution in question depends on several free parameters: ρ_*, $const$, d_1, and d_2 (see (3.25), (4.2.2), and

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(5.1.2), respectively). Moreover, $\overset{(2)}{\sigma}_{zz}$ from (3.26.2) depends on $\mathcal{C}\ (= Q')$. In order to avoid the arbitrariness, the asymptotical stresses should be subject to appropriate conditions at $\kappa\rho \gg 1$ and $\kappa\rho \ll 1$. For instance, $I_{\mathcal{F}}$ is exponentially small for $\kappa\rho \gg 1$, and therefore $f \simeq f_{\mathrm{bg}}(\rho)$. As a result, $\overset{(2)}{\sigma}_{\rho\rho} \simeq (\overset{(2)}{\sigma}_{\mathrm{bg}})_{\rho\rho}$ and $\overset{(2)}{\sigma}_{\phi\phi} \simeq (\overset{(2)}{\sigma}_{\mathrm{bg}})_{\phi\phi}$, where the background stresses are given by (5.4). However, d_1 and d_2 in the gauge case are defined below.

In the limit $\kappa\rho \ll 1$, we use (4.7) and (5.1) and obtain $\overset{(2)}{\sigma}_{\rho\rho}$ and $\overset{(2)}{\sigma}_{\phi\phi}$ as follows:

$$
\overset{(2)}{\sigma}_{\rho\rho} - (\overset{(2)}{\sigma}_{\mathrm{bg}})_{\rho\rho} \simeq \ - \ 2r_2\frac{\log\rho}{\rho^2} - \frac{r_1}{\rho^2} - 2r_3\log^3\rho - (3r_3 + 2r_4)\log^2\rho
$$

$$
- \ 2(r_4 + r_5)\log\rho - (r_5 + 2r_6) - 4r_7\rho^2\log^3\rho + \dots ,
$$

$$
\overset{(2)}{\sigma}_{\phi\phi} - (\overset{(2)}{\sigma}_{\mathrm{bg}})_{\phi\phi} \simeq \ \ 2r_2\frac{\log\rho}{\rho^2} - \frac{2r_2 - r_1}{\rho^2} \tag{5.8}
$$

$$
- \ 2r_3\log^3\rho - (9r_3 + 2r_4)\log^2\rho - 2(3r_3 + 3r_4 + r_5)\log\rho
$$

$$
- \ (3r_5 + 2r_4 + 2r_6) - 12r_7\rho^2\log^3\rho + \dots ,
$$

where the background stresses on the left-hand side are given by (5.4). Now, r_1, r_2, ..., and r_7 include, for notational compactness, the multiple k from (5.1.1). The contributions $\propto \rho^{-2}\log\rho$ disappear on both sides of (5.8) since r_2 is equal to $\widetilde{n}$. The contributions due to r_3 and r_7 disappear in (5.8) since $p_2 = 0$ in (3.31). However, the terms, which are either divergent or constant as $\rho \to 0$, are still contained in (5.8).

The number of the free parameters is smaller in comparison with [50] since now $C = 0$ in (4.6). Therefore, the inappropriate terms in (5.8) should be handled differently. Recall that the core region corresponds to $\rho \lesssim \kappa^{-1}$. Let us introduce a fictitious boundary at $\rho = \rho_\varepsilon$, where $\rho_\varepsilon \ll \kappa^{-1}$. We assume that ρ varies within the segment $[\rho_\varepsilon, \rho_\mathrm{e}]$, where ρ_ε is allowed to be arbitrarily small but strictly non-zero. Then we arrive at the following equations:

$$
\frac{r_1 + d_2}{\rho_\varepsilon^2} + 2r_4\log^2\rho_\varepsilon + 2(r_4 + r_5)\log\rho_\varepsilon + r_5 + 2(r_6 + d_1) = 0 ,
$$

$$
\frac{r_1 + d_2}{\rho_\varepsilon^2} - 2r_4\log^2\rho_\varepsilon - 2(3\,r_4 + r_5)\log\rho_\varepsilon - 3\,r_5 - 2(r_4 + r_6 + d_1) = 0 , \tag{5.9}
$$

$$
2\widetilde{n}\log\rho_\mathrm{e} - d_2 - 2\rho_\mathrm{e}^2\,d_1 = 0 .
$$

The first two equations in (5.9) imply that the terms, which are either divergent or constant in (5.8), vanish at $\rho = \rho_\varepsilon$. Therefore, $\overset{(2)}{\sigma}_{\rho\rho}$ and $\overset{(2)}{\sigma}_{\phi\phi}$ at $\rho = \rho_\varepsilon$ are mainly given by the terms that go to zero as $\rho_\varepsilon \to 0$. The third equation in (5.9) reads that the radial stress is zero at the outer boundary $\rho = \rho_\mathrm{e}$. The arbitrariness of d_1, d_2, and $const$ can be used to meet (5.9). Since d_1, d_2, and $const$ are thus determined (as functions of ρ_ε, in fact), we can use them in (5.1) and (5.3) to produce the stress distribution valid on the ring, say, $\mathcal{D}_{[\rho_\varepsilon,\rho_\mathrm{e}]}$ confined between $\rho = \rho_\varepsilon$ and $\rho = \rho_\mathrm{e}$.

Let us consider an infinite sequence of concentric circles with monotonically decreasing radii $\rho = \rho_\varepsilon$ (ρ_ε's remain however non-zero). Each of the corresponding rings $\mathcal{D}_{[\rho_\varepsilon,\rho_\mathrm{e}]}$ is completely covered by a disc with the same external boundary $\rho = \rho_\mathrm{e}$ but with a puncture at $\rho = 0$. The stress distributions defined on the rings also form a sequence. It can naturally be considered as converging to an appropriate solution defined on the punctured disc. Such

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a limit is expected to exist, since the boundary values $\overset{(2)}{\sigma}_{ij}\Big|_{\rho=\rho_\varepsilon}$ go to zero for decreasing ρ_ε. Therefore, our attention is focussed at the rings possessing sufficiently small internal radii. Note that even the definition (4.2) is concerned with a hollow domain possessing a sufficiently small internal radius. It is just the regularization in (4.2), which allows us to send this radius to zero immediately.

To extract the dependence on *const* in (5.9), let us turn to q_4 and q_5 from (4.4). Using Appendix B, one can establish that r_1 in (4.8) and r_5, r_6 in (B11) depend on *const* as follows:

$$r_1 \equiv -\widetilde{C} + \widetilde{r}_1, \quad r_5 \equiv -\frac{\kappa^2}{4}\widetilde{C} + \widetilde{r}_5, \quad r_6 \equiv \frac{q\,\kappa^2}{4}\widetilde{C} + \widetilde{r}_6. \tag{5.10}$$

The following notation is accepted in (5.10):

$$\widetilde{C} \equiv \text{const} \times \frac{k}{\kappa^2 + \mathcal{N}^2}, \quad q \equiv 1 - \log\left(\frac{\gamma}{2}\kappa\right), \tag{5.11}$$

where $\kappa^2 = \mu/\ell$ (μ is the shear modulus, and ℓ arises in (2.10)) and $(\kappa/\mathcal{N})^2 = 1 - 2a$. Moreover, a and k are given by (3.10) and (3.21), respectively. We substitute (5.10) into (5.9) and rewrite the result as a single 3×3 matrix equation:

$$\begin{pmatrix} a & 0 & 1 \\ b & 2\rho_\varepsilon^2 & 1 \\ 0 & 2\rho_e^2 & 1 \end{pmatrix} \begin{pmatrix} \widetilde{C} \\ d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} l_1 \\ l_2 \\ l_3 \end{pmatrix}, \tag{5.12}$$

where

$$a \equiv -1 + \frac{(\kappa\rho_\varepsilon)^2}{4},$$

$$b \equiv -1 - \frac{(\kappa\rho_\varepsilon)^2}{2}\left(\frac{1}{2} - q + \log\rho_\varepsilon\right),$$

$$l_1 \equiv 2r_4\rho_\varepsilon^2 \log\rho_\varepsilon + (r_4 + \widetilde{r}_5)\rho_\varepsilon^2 - \widetilde{r}_1, \tag{5.13}$$

$$l_2 \equiv -2r_4\rho_\varepsilon^2 \log^2\rho_\varepsilon - 2(r_4 + \widetilde{r}_5)\rho_\varepsilon^2 \log\rho_\varepsilon - (\widetilde{r}_5 + 2\widetilde{r}_6)\rho_\varepsilon^2 - \widetilde{r}_1,$$

$$l_3 \equiv 2\widetilde{n}\log\rho_e.$$

Equation (5.12) is solved for d_1, d_2, and $\widetilde{C}$ by the Cramer's rule:

$$\widetilde{C} = \frac{2}{\mathcal{D}}\left(\rho_e^2(l_2 - l_1) + \rho_\varepsilon^2(l_1 - l_3)\right),$$

$$d_1 = \frac{1}{\mathcal{D}}\left(al_2 - bl_1 + l_3(b - a)\right), \tag{5.14}$$

$$d_2 = \frac{2}{\mathcal{D}}\left(\rho_e^2(bl_1 - al_2) + \rho_\varepsilon^2 al_3\right),$$

where $\mathcal{D} \equiv 2a\rho_e^2 + 2(b - a)\rho_\varepsilon^2$. The parameters $\widetilde{C}$ (i.e., *const*, see (5.11)), d_1, and d_2 thus obtained should be used in f from (5.1).

Let us assume that ρ_ε is sufficiently small (the so-called *logarithmic approximation*):

$$1 \ll \kappa \ll \frac{1}{\rho_\varepsilon} \ll \frac{1}{\rho_\varepsilon}\log\frac{1}{\rho_\varepsilon}. \tag{5.15}$$

Then, the ratios (5.14) can be represented in the perturbative form

$$\widetilde{C} \simeq -\frac{4r_4}{\kappa^2} \log \frac{1}{\rho_\varepsilon} + \frac{4}{\kappa^2}\Big(\widetilde{r}_5 + (1+q)\,r_4\Big) + \dots \,,$$

$$d_1 \simeq \frac{1}{\rho_e^2}\Big(\widetilde{n}\log\frac{\rho_e}{\rho_1} + 2\frac{r_4}{\kappa^2}\log\frac{1}{\rho_\varepsilon}\Big) + \dots \,, \qquad (5.16)$$

$$d_2 \simeq -4\frac{r_4}{\kappa^2}\log\frac{1}{\rho_\varepsilon} - 2\widetilde{n}\log\frac{1}{\rho_1} + \dots \,,$$

where dots imply terms that tend to zero as $\rho_\varepsilon \to 0$. In addition, the new length parameter ρ_1 is intended to express the contributions which are constant as $\rho_\varepsilon \to 0$:

$$2\widetilde{n}\,\log\frac{1}{\rho_1} \equiv \widetilde{r}_1 - \frac{4}{\kappa^2}\Big(\widetilde{r}_5 + (1+q)\,r_4\Big), \qquad (5.17)$$

where q is given by (5.11). Using (5.4) and (5.16), we obtain sufficiently far from the core:

$$\overset{(2)}{\sigma}_{\rho\rho} \approx \frac{2\widetilde{n}}{\rho^2}\Big(\log\frac{\rho}{\rho_1} - \Big(\frac{\rho}{\rho_e}\Big)^2\log\frac{\rho_e}{\rho_1}\Big) - 4\frac{r_4}{\kappa^2}\log\rho_\varepsilon\Big(\frac{1}{\rho^2} - \frac{1}{\rho_e^2}\Big),$$

$$\overset{(2)}{\sigma}_{\phi\phi} \approx \frac{2\widetilde{n}}{\rho^2}\Big(1 - \log\frac{\rho}{\rho_1} - \Big(\frac{\rho}{\rho_e}\Big)^2\log\frac{\rho_e}{\rho_1}\Big) + 4\frac{r_4}{\kappa^2}\log\rho_\varepsilon\Big(\frac{1}{\rho^2} + \frac{1}{\rho_e^2}\Big). \qquad (5.18)$$

As far as the asymptotic expansions (5.18) are concerned, it is crucial that r_4 can be made equal to zero. Indeed, using r_4 in the form (4.8) (where p_1 and p_3 from (3.32) are used, and p_2 is zero), we obtain ρ_*^2 from the equation $r_4 = 0$ as follows:

$$\rho_*^2 = \frac{B(\eta,\alpha)}{\kappa^2}\,, \qquad B(\eta,\alpha) \equiv \frac{8(1-\nu)(1-\eta)}{\alpha(1-\nu)\eta - 2\nu(1-\eta)}\,,$$

$$\eta \equiv 4(1+\nu)\,\frac{\mu^2 C_3}{1 - 2\mu^2 C_7}\,, \qquad (5.19)$$

where $\alpha = 1$ or $\alpha = 3$, according to (3.32). Equations (5.19) lead to the positivity of the coefficient-function $B(\eta,\alpha)$. The validity of (3.24) holds better whenever κ^{-1} and ρ_* are smaller. If the scale κ^{-1} is small enough, a bound B_0 can be found to restrict $B(\eta,\alpha)$: $0 < B(\eta,\alpha) \lesssim B_0$. If so, ρ_* from (5.19) is estimated as $\rho_* = O(\kappa^{-1})$. In terms of η, the corresponding restriction takes the form

$$\Big(1 + \frac{\alpha}{2}\frac{1-\nu}{\nu}\Big)^{-1} < \big(1+U\big)^{-1} \lesssim \eta < 1\,, \qquad U \equiv \frac{\alpha(1-\nu)B_0}{8(1-\nu) + 2\nu B_0}\,, \qquad (5.20)$$

where $0 < \nu \le 1/2$ for isotropic materials.

It is straightforward to rewrite (5.20) in terms of the elastic parameters C_3 and C_7:

$$a) \quad C_7 + 2(1+\nu)\,C_3 < \frac{1}{2\mu^2} \lesssim C_7 + 2\,(1+\nu)\big(1+U\big)\,C_3\,, \qquad C_3 > 0\,,$$

$$\qquad (5.21)$$

$$b) \quad C_7 + 2\,(1+\nu)\big(1+U\big)\,C_3 \lesssim \frac{1}{2\mu^2} < C_7 + 2(1+\nu)\,C_3\,, \qquad C_3 < 0\,.$$

Further, (5.21) can be re-expressed [7] in terms of the parameters m' and n' from (3.4), which can in turn be related [4] to the third order elastic moduli of the cubic crystals. In other

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words, the choice of material is restricted by (5.21). The numerical data provided by [4] witness that these conditions look realistic for certain materials. However, to discuss (5.21) from the viewpoint of real crystallography is beyond the scope of the present investigation.

Straightforward usage of (4.6), (5.1), and (5.3) leads us to the following general expression for the stress components:

$$
\begin{aligned}
\overset{(2)}{\sigma}_{\rho\rho} &= (\overset{(2)}{\sigma}_{\text{far}})_{\rho\rho} - k\,\rho^{-1}I'_{\mathcal{F}}\,, \\[2mm]
\overset{(2)}{\sigma}_{\phi\phi} &= (\overset{(2)}{\sigma}_{\text{far}})_{\phi\phi} + k\big(\mathcal{N}^2 I_{\mathcal{F}} + \rho^{-1}I'_{\mathcal{F}} - G\big)\,,
\end{aligned}
\tag{5.22}
$$

where k and G are given by (3.21) and (4.2), correspondingly, and $I'_{\mathcal{F}}$ (the prime implies the differentiation $d/d\rho$) is expressed as follows:

$$
\mathcal{N}^{-1}I'_{\mathcal{F}} = \widetilde{Y}_1(\mathcal{N}\rho)\int_\rho^\infty J_0(\mathcal{N}t)G(\kappa t)\,t\,dt - J_1(\mathcal{N}\rho)\int_\rho^\infty \widetilde{Y}_0(\mathcal{N}t)G(\kappa t)\,t\,dt\,.
$$

It is assumed that $\widetilde{Y}_1(\cdot) \equiv (\pi/2)Y_1(\cdot)$ (similar to $\widetilde{Y}_0$ in (4.6)). Now, the subscript 'far' labels the stress components in (5.22) in order to emphasize the non-conventional choice of d_1 and d_2, which corresponds to (5.16), provided that the internal radius of the ring $\mathcal{D}_{[\rho_\varepsilon,\rho_e]}$ is small enough. We also obtain the sum of the second order stress components:

$$
\overset{(2)}{\sigma}_{\rho\rho} + \overset{(2)}{\sigma}_{\phi\phi} = (\overset{(2)}{\sigma}_{\text{far}})_{\rho\rho} + (\overset{(2)}{\sigma}_{\text{far}})_{\phi\phi} + k\big(\mathcal{N}^2 I_{\mathcal{F}} - G\big)\,.
\tag{5.23}
$$

Since r_4 is zero for ρ_*^2 from (5.19), the limit $\rho_\varepsilon \to 0$ is suitable in (5.16) to eliminate ρ_ε. Then, d_1 and d_2 acquire the classically known form (5.6), though ρ_1 is present instead of ρ_c. The limiting value of the parameter *const* (see (4.2)) is also expressed with the help of (5.11) and (5.16), provided that ρ_ε decreases to zero. The large-distance stresses (5.18) take at $r_4 = 0$ the classical form (5.7). Note that the axis Oz is not captured by the present approach, as far as the limiting transition is allowed. This is in agreement with the regularization of the density profile at $\rho = 0$ in Section 3. The components $(\overset{(2)}{\sigma}_{\text{far}})_{\rho\rho}$ and $(\overset{(2)}{\sigma}_{\text{far}})_{\phi\phi}$ reduce, after the shrinking of the internal boundary of the ring, to (5.18) (with r_4 equated to zero) and should be distinguished from the analogous ones given by (5.7). Eventually, there is no cut-off around the dislocation's core for the second order stresses expressed by (5.22), provided that the numerical parameters are substituted appropriately.

5.2 The component σ_{zz}

Let us consider the stress component $\overset{(2)}{\sigma}_{zz} = p$. Classically, the second equation in (3.20) implies the following representation [7]:

$$
\overset{(2)}{\sigma}_{zz} = \nu\big(\overset{(2)}{\sigma}_{\rho\rho} + \overset{(2)}{\sigma}_{\phi\phi}\big) - 2\mu(1+\nu)\big(\Psi_{zz}^{\text{bg}} + Q'\big)\,,
\tag{5.24}
$$

where f_{bg} from (5.1.2) is used for the stresses on the right-hand side (the respective subscript is omitted for brevity), and $\overset{(1)}{\phi}_{\text{bg}} = (-b/2\pi)\log\rho$ is substituted to express Ψ_{zz}^{bg}. As far as the equation (5.24) is concerned, it is assumed that the argument ρ varies within the segment

$[\rho_c, \rho_e]$, and Q' is determined from the requirement that $\overset{(2)}{\sigma}_{zz}$ averaged over $\mathcal{D}_{[\rho_c,\rho_e]}$ is zero (the so-called 'mean stress theorem'; see [4]). Then, the representation (5.24) reads for $\rho_e \gg \rho_c$:

$$\overset{(2)}{\sigma}_{zz} \approx 2\left[\nu\widetilde{n} + \left(\frac{b}{2\pi}\right)^2 \mu^3(1+\nu)C_3\right]\left[\frac{1}{\rho^2} - \frac{2}{\rho_e^2}\log\frac{\rho_e}{\rho_c}\right]. \tag{5.25}$$

Let us turn to the stress component $\overset{(2)}{\sigma}_{zz}$ from (3.26.2) of the modified defect:

$$\overset{(2)}{\sigma}_{zz} = \nu\left(\overset{(2)}{\sigma}_{\rho\rho} + \overset{(2)}{\sigma}_{\phi\phi}\right) - 2\mu(1+\nu)(\Psi_{zz} + \widetilde{g}) + \kappa^2(1+\nu)(f - f_{\rm bg}). \tag{5.26}$$

Now ρ varies within $[\rho_\varepsilon, \rho_e]$. From the previous considerations it is clear that $\overset{(2)}{\sigma}_{\rho\rho} + \overset{(2)}{\sigma}_{\phi\phi}$ and Ψ_{zz}, taken at $\rho = \rho_\varepsilon$, decrease as $\rho_\varepsilon \to 0$. Nevertheless, $\overset{(2)}{\sigma}_{zz}$ behaves, sufficiently close to Oz, somewhat artificially. The reason is that the logarithmic terms dominate in $f - f_{\rm bg}$ at ρ small enough. However, this is not an obstacle to view the rings $\mathcal{D}_{[\rho_\varepsilon,\rho_e]}$, as well as (in the limiting sense) the punctured disc, as the domains of definition of the stress distributions. Indeed, $\overset{(2)}{\sigma}_{zz}$ from (5.26), averaged over $\mathcal{D}_{[\rho_\varepsilon,\rho_e]}$, is finite, provided that ρ_ε goes to zero.

Let us obtain $\overset{(2)}{\sigma}_{zz}$ from (5.26) at sufficiently large distances, where $f - f_{\rm bg} (= kI_{\mathcal{F}})$ is exponentially small. Using (5.18) at $r_4 = 0$, we obtain

$$\overset{(2)}{\sigma}_{zz} \approx 2\nu\widetilde{n}\left[\frac{1}{\rho^2} - \frac{2}{\rho_e^2}\log\frac{\rho_e}{\rho_1}\right] - 2\mu(1+\nu)\left[Q' - \left(\frac{b}{2\pi}\right)^2\frac{c}{\rho^2}\right]. \tag{5.27}$$

We determine Q' approximately:

$$Q' \approx \left(\frac{b}{2\pi}\right)^2 2c\frac{\log(\rho_e/\rho_2)}{\rho_e^2}, \tag{5.28}$$

where another length ρ_2 is introduced, namely,

$$\begin{aligned}
\left(\frac{b}{2\pi}\right)^2 2c\log\frac{1}{\rho_2} &\equiv \left(\frac{b}{4\pi}\right)^2 - 2\int_0^1 \Psi_{zz}\,\rho\,d\rho \\
&\quad - 2\int_1^\infty\left[\Psi_{zz} + \left(\frac{b}{2\pi}\right)^2\frac{c}{\rho^2}\right]\rho\,d\rho + 2\kappa^2\frac{1+\nu}{1-\nu}\int_0^\infty I_{\mathcal{F}}\,\rho\,d\rho,
\end{aligned} \tag{5.29}$$

provided that $\rho_\varepsilon \to 0$, and the upper integration bound ρ_e is replaced approximately by infinity.

Therefore, (5.27) depends on two scales, which are, in principle, different in our consideration: ρ_1 from (5.17) and ρ_2 from (5.29). To re-write (5.27) more conventionally, it is appropriate to introduce another length, say ρ_m, as follows:

$$\begin{aligned}
\left[\nu\widetilde{n} + \left(\frac{b}{2\pi}\right)^2\mu(1+\nu)c\right]&\log\frac{1}{\rho_m} \\
&\equiv \nu\widetilde{n}\log\frac{1}{\rho_1} + \left(\frac{b}{2\pi}\right)^2\mu(1+\nu)c\log\frac{1}{\rho_2}.
\end{aligned} \tag{5.30}$$

Substituting Q' from (5.28) into (5.27) and using (5.30), we obtain

$$\overset{(2)}{\sigma}_{zz} \approx 2\left[\nu\widetilde{n} + \left(\frac{b}{2\pi}\right)^2\mu(1+\nu)c\right]\left[\frac{1}{\rho^2} - \frac{2}{\rho_e^2}\log\frac{\rho_e}{\rho_m}\right]. \tag{5.31}$$

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Equation (5.31) looks similarly to (5.25), except that now $\rho_{\rm m}$ is present instead of $\rho_{\rm c}$.

The classical answers for d_1 and d_2 are given at $\rho_{\rm e} \gg \rho_{\rm c}$ by (5.6). Since d_1 and d_2 from (5.16) include the constant contributions, the agreement between (5.6) and (5.16) is due to the newly defined length ρ_1 from (5.17). The mean stress theorem implies that ρ_2 coincides, classically, with the lower integration boundary $\rho_{\rm c}$, provided that $\rho_{\rm c}$ remains unspecified. Instead, Q' in (5.28) is concerned with another length ρ_2 from (5.29). This is because Ψ_{zz} is unconventional inside the core. In the present approach, two different lengths arise. The definition (5.30) is only to obtain the classically-looking representation (5.31).

We use $\widetilde{g}$ (3.25), where $\mathcal{C} = Q'$ with Q' given by (5.28), and we rewrite the stress $\overset{(2)}{\sigma}_{zz}$ expressed by (5.26):

$$
\begin{aligned}
\overset{(2)}{\sigma}_{zz} \;=\;& \nu\left(\overset{(2)}{\sigma}_{\rho\rho} + \overset{(2)}{\sigma}_{\phi\phi}\right) - 2\mu\,(1+\nu)\left[\Psi_{zz} - \frac{2}{\rho_{\rm e}^2}\int_0^{\rho_{\rm e}}\Psi_{zz}\,\rho\,d\rho\right] \\[2mm]
& - 2\mu\,(1+\nu)\left(\frac{b}{4\pi}\right)^2\left[\frac{1}{\rho_{\rm e}^2} + \frac{2}{\rho_*^2}\left(\frac{\rho^2}{\rho_*^2} - 1\right)h_{[0,\rho_*]}(\rho)\right] \\[2mm]
& + 2\kappa^2\,\frac{\mu(1+\nu)^2}{1-\nu}\left[I_{\mathcal{F}} - \frac{2}{\rho_{\rm e}^2}\int_0^{\rho_{\rm e}}I_{\mathcal{F}}\,\rho\,d\rho\right].
\end{aligned}
\tag{5.32}
$$

Moreover, using (5.23) we can further rewrite (5.32) for sufficiently large $\rho_{\rm e}$ as follows:

$$
\begin{aligned}
\overset{(2)}{\sigma}_{zz} \;\approx\;& \nu\left((\overset{(2)}{\sigma}_{\rm far})_{\rho\rho} + (\overset{(2)}{\sigma}_{\rm far})_{\phi\phi}\right) - 2\mu\,(1+\nu)\Psi_{zz} \\[2mm]
& - 2\mu\,(1+\nu)\left(\frac{b}{2\pi}\right)^2\left[\frac{2c}{\rho_{\rm e}^2}\log\frac{\rho_{\rm e}}{\rho_2} + \frac{1}{2\rho_*^2}\left(\frac{\rho^2}{\rho_*^2} - 1\right)h_{[0,\rho_*]}(\rho)\right] \\[2mm]
& + k\left(\mathcal{N}^2 I_{\mathcal{F}} - \nu\,G\right),
\end{aligned}
\tag{5.33}
$$

where k, G, $I_{\mathcal{F}}$, and ρ_*^2 are given by (3.21), (4.2), (4.6), and (5.19), respectively. Expression for Ψ_{zz} from (3.18) in the polar coordinates takes the form: $\Psi_{zz} = -c(\partial_\rho\,\overset{(1)}{\phi})^2$, where $\overset{(1)}{\phi}$ is given by (3.13). The behaviour of Ψ_{zz} for sufficiently large distances is similar to that of $\Psi_{zz}^{\rm bg}$ although is different within the core.

Let us recall that a stationary Schrödinger equation obtained in the effective mass approximation [63] has been used for the conduction electrons in the dislocated [13] or disclinated crystals [44], [45]. The influence of the defects has been accounted for via the deformation potential given by the trace of the strain tensor (i.e., by the dilatation). The gauge and/or geometric approaches to various effects due to the dislocations (due to the torsion) attract considerable attention: [64]– [70], [72], and [73][4].

The dilatation is non-trivial for the screw dislocation just because of the strains of the second order. Sufficiently far from the core, the dilatation depends on $1/\rho^2$ just by means of m' and n' from (3.4) (see [7]). The results obtained above can be applied to the Schrödinger equation, as is discussed in [13]. Indeed, the solution [13] is valid only outside the core, and, say, a traction-free condition is still required. In turn, a possible influence of the dilatation, obtainable by the present approach, on a local shape of the wave function can be investigated in the vicinity of the core region. The corresponding results should be comparable with appropriate lattice-based investigations. Note that the disclination core's radii have been used in [44] and [71] for description of the corresponding electron localization.

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[4]For more refs. on other types of defects, see [57].

5.3 Remarks on the logarithmic approximation

The asymptotic relations (5.16) give an indication of the fact that the ratios (5.14) should be re-arranged perturbatively for $\log(1/\rho_\varepsilon)$ and ρ_e sufficiently large. It is instructive to re-derive the leading terms in (5.16) by means of a more straightforward use of the logarithmic approximation at $r_4 = 0$. Indeed, let us reconsider (5.12), provided that the parameters (5.13) are taken in the principal order as follows:

$$a \approx -1, \qquad b \approx -1 - \frac{(\kappa\rho_\varepsilon)^2}{2} \log \rho_\varepsilon,$$

$$l_1 \approx -\widetilde{r}_1, \qquad l_2 \approx -\widetilde{r}_1 - 2\overset{\circ}{r}_5 \rho_\varepsilon^2 \log \rho_\varepsilon. \tag{5.34}$$

Here, $r_4 = 0$ in $\widetilde{r}_1$, and the special notation $\overset{\circ}{r}_5$ is chosen for $\widetilde{r}_5$ at $r_4 = 0$. Besides, l_3 is kept like in (5.13). We replace in (5.12) the entry equal to $2\rho_\varepsilon^2$ by zero. Then, in agreement with (5.16), the solution reads:

$$\widetilde{C} = \frac{4\overset{\circ}{r}_5}{\kappa^2}, \qquad d_1 = \frac{\widetilde{n}}{\rho_e^2} \log \frac{\rho_e}{\rho_1}, \qquad d_2 = 2\widetilde{n} \log \rho_1, \tag{5.35}$$

where ρ_1 agrees with (5.17).

Moreover, one can estimate ρ_1, provided that $\log \kappa$ is large enough. With regard to the definition by means of the equation (5.10), we extract the dependence of $\widetilde{r}_1$ and $\widetilde{r}_6$ on the large logarithm as follows (r_4 is zero):

$$\widetilde{r}_1 = \frac{q_1}{\kappa^2} \log \kappa + \overset{\circ}{r}_1, \qquad \widetilde{r}_6 = \overset{\circ}{r}_5 \log \kappa + \overset{\circ}{r}_6. \tag{5.36}$$

The terms $\overset{\circ}{r}_1$ and $\overset{\circ}{r}_6$ in (5.36) are simply intended to denote the corresponding remnants, which are finite, provided that $\log \kappa$ is growing. We can use (5.36) in (5.13) and again directly solve (5.12). Then, d_1 and d_2 appear just in the form (5.35) with $\rho_1 = B_1/\kappa$, where

$$2\widetilde{n} \log B_1 \equiv -\overset{\circ}{r}_1 + \frac{4}{\kappa^2} \overset{\circ}{r}_5. \tag{5.37}$$

It is seen that (5.37) agrees with (5.17). The radius ρ_2 can also be estimated. From (5.29) we obtain $\rho_2 = B_2/\kappa$, where

$$2c \log B_2 \equiv -\frac{1}{4} - 2c \int_0^1 (1 - s\,K_1(s))^2 \frac{ds}{s}, \tag{5.38}$$

and c is given by (3.30). Therefore, the logarithmic approximation allows us to determine the leading behaviour of $\widetilde{C}$, d_1, and d_2, as well as to estimate ρ_1 and ρ_2. Note in passing that a certain influence of the regularization in (4.2) on B_1 from (5.37) and B_2 from (5.38) should be accounted for, though elsewhere (since specific numerical estimates based on the crystallographic data are required).

The result (5.35) should be commented as follows. Let us introduce a sufficiently small positive $\in$ by the requirement: absolute values of the stresses, which are smaller than $\in$ (say, $|\overset{(2)}{\sigma}_{ij}| \leq \frac{\in}{2}$), should be treated, for engineering, as indistinguishable from zero. Then, the

shrinking of the boundary at $\rho = \rho_\varepsilon$ can be ceased just for those boundary values $\overset{(2)}{\sigma}_{ij}\Big|_{\rho=\rho_\varepsilon}$, which respect this estimate. At the same time, (5.15) holds, and thus (5.35), (5.37), and (5.38) are valid. The large distance behavior looks conventional though includes now ρ_1 and ρ_2, which are dictated by a choice of material. Provided ρ_ε is thus fixed, the stress $\overset{(2)}{\sigma}_{zz}$ remains bounded outside an infinitesimally thin tube around Oz. It is essential that under the prescribed accuracy $\in$, a distant "observer" outside the core is dealt only with the physical stresses improved by means of ρ_1 and ρ_2. These stresses are insensitive to particular ρ_ε's.

Let us turn again to our geometric interpretation. Let us imagine for a moment that the differential-geometric torsion is taken into account in order to make (3.16) conventionally looking. Then, $\Delta \overset{(1)}{\phi}_{\mathcal{T}}$ comes to play instead of $\Delta \overset{(1)}{\phi}$. Since a specific shape of appropriately localized density $\mathcal{T}$ is unclear, (3.24) can be applied, as a simplification, just to $\Delta \overset{(1)}{\phi}_{\mathcal{T}}$. As a result, the driving source $\mathcal{R}$ should be changed. The local properties of this new $\mathcal{R}$ can be estimated. The modifications are expectable for p_4, p_5, and p_6 from (3.31). However, these changes do not influence the coefficients we consider in (4.7). A change of shapes of the profiles of the stress components is expectable in the middle of the core, but this is beyond our scope. It is important that ρ_1 in (5.17) and ρ_* in (5.19) should not be influenced when $\Delta \overset{(1)}{\phi}_{\mathcal{T}}$ is subject to (3.24). Only ρ_2 from (5.29) should be replaced, since it is defined "globally". Thus, the present picture is almost the same as that with the torsion admitted but handled approximately. To avoid a specification of $\mathcal{T}$, it is appropriate to keep our teleparallel interpretation.

6 Discussion

The stress potential of the non-singular screw dislocation is found in the quadratic approximation. It is given by the sum of the conventional part and the gauge contribution. The general expression (5.22) for the stress components of second order $\overset{(2)}{\sigma}_{\rho\rho}$ and $\overset{(2)}{\sigma}_{\phi\phi}$ is also obtained by means of appropriate differentiations of the stress potential. In addition, the general expression for the stress $\overset{(2)}{\sigma}_{zz}$ is elaborated as well: see, for instance, (5.32) or (5.33). The main attention is paid to the asymptotic properties of the stresses in question. To ensure their self-consistency, the arbitrariness of certain constants in the general solution for the stress potential is used.

Sufficiently far from the core, the second order stresses obtained, $\overset{(2)}{\sigma}_{\rho\rho}$, $\overset{(2)}{\sigma}_{\phi\phi}$, and $\overset{(2)}{\sigma}_{zz}$ are in agreement with [7], although now they include the new lengths ρ_1 and ρ_2. The non-conventional part of the total stress potential is responsible for the localized contribution into the full stress distribution. As a result, the modification of the short-distance behaviour is as follows: $\overset{(2)}{\sigma}_{\rho\rho}$ and $\overset{(2)}{\sigma}_{\phi\phi}$ tend to zero, while $\overset{(2)}{\sigma}_{zz}$ grows logarithmically (although $\overset{(2)}{\sigma}_{zz}$ is integrable, as required in [7]) in the close vicinity of Oz. There is no artificial cut-off at an internal boundary. The "exterior" (with respect to the core region) solution for the second-order stresses plays a central role in the picture presented. This is because of its improvement due to the self-consistent arising of ρ_1 and ρ_2. The general solution is characterized by one more length ρ_* which is a half-width of the effective defect's density profile.

The lengths ρ_1, ρ_2, and ρ_* are expressed through the elastic moduli of second and third

order. The appearance of several lengths correlates with the absence of a sharp boundary around the core in the first order pictures in [14], [15], [17], and [19]. In other words, a concept of 'transition shell' looks helpful for characterization of the solution obtained. This shell would separate two domains: a compact region under the shell, where the strains are rather finite, and an outer bulk. The solution obtained should be less reliable under the shell (where the effects of discreteness are comparable with those of strong elastic non-linearity; see [3] and [4]). Within the transition shell, the quadratic corrections both of the conventional and of the gauge origin (i.e., due to $I_{\mathcal{F}}$ in the stress potential) should be important. Outside the shell (i.e., in the bulk), the conventional terms become more valuable, since the gauge contributions are strongly decaying. The radii obtained ρ_1, ρ_2, and ρ_* should characterize the location and the extent of the transition shell. More generally, they seem to display the dislocation cores as radially-layered regions.

The radii ρ_*, ρ_1, and ρ_2 include the basic length $1/\kappa$ ($\equiv \sqrt{\ell/\mu}$), which can be adjusted to the interatomic scale even in the first order: see, for instance, [14] and [17]. Analogous identifications can also be found in [20], [24], and [26]. Here ℓ is the gauge-material parameter (see (2.10)) and μ is the shear modulus. However, the corresponding coefficients $B(\eta, \alpha)$, B_1, and B_2 given by (5.19), (5.37), and (5.38), respectively, are strictly influenced by the crystallographic moduli of second and third order. Mutual comparisons of the coefficients and more specific statements on the properties of the transition shell should be done elsewhere. The numerically obtainable values for ρ_1, ρ_2, and ρ_* can be compared, in principle, with appropriate scales provided by the semi-discrete models of the cores (see refs. in [3], [4], and [10]). On the other hand, attempts at matching the radii in accordance with the experimental observations may result in independent estimate for $1/\kappa$. Such estimate can, in turn, be compared with $1/\kappa$ obtainable by means of the first-order considerations.

As far as the numerical estimates are concerned, the isotropy requirement should be taken into account, since the number of the elastic constants of third order for the cubic crystals is six (see [4] and [10]). Moreover, strong couplings could modify the elastic parameters within the core in comparison with those outside it (see [40]). Note that [36] also provides the radius of the screw dislocation as a function of the elastic constants (of second order though) and of the lattice spacings of the crystal.

Strains and displacements within the transition shell can, in principle, be elaborated with the help of the present approach. For instance, the displacements of the first order in the core region are discussed in [14] and [17]. The next order corrections to those displacements can be obtained within the shell. Here, the technical issue [74] could be helpful. Thus corrected displacements should be comparable with the semi-discrete calculations subject to the so-called flexible boundary conditions (see [75] and [76]). Direct observations of the dislocation cores by means of the high resolution electron microscopy can also be used for comparison (for more refs. on the observation and modelling of the dislocation cores at atomic level in semiconductors, for instance, see [78]). The solution obtained can also be tested for the problems where just the second-order elasticity is relevant, e.g., for the elastic waves or the electron (see Sec. 5.2) scattering, etc. (see [4] and [9]).

The continuation obtained for the stresses is just due to the gauge equation considered as the incompatibility law. In turn, our constitutive equations imply that the elastic energy is written up to the third order. But the quadratic constitutive law is only an approximation for essentially non-linear situation. Clearly, the present picture does not pretend to simulate the stress distribution in the middle of the core, where both the atomistic structure and the finite elasticity are crucial (see [77] where a non-linear elasticity approach with flexible boundary is discussed as a way for improving the semi-discrete techniques). Nevertheless, the

stress distribution provided by the present model of the screw dislocation is self-contained outside a certain shell, and it seemingly remains satisfactory within this shell as well.

Our investigation demonstrates that the Hilbert–Einsteinian gauge approach is flexible enough, since it allows, in two orders, the self-consistent description for the non-singular screw dislocation. Certain features of an extended picture could be discovered in the present model. It can be used as a base for further, more involved, treatments. Application to the edge dislocation would be also desirable.

Acknowledgement

Appendix A

Appendices A and B contain intermediate results, which are helpful for expanding the stress potential f in (5.1) (see also [50]). Starting with the series expansion (3.31) and using the Bessel functions in the series form [59], we go over to the corresponding series $\mathcal{F}$ from (4.7).

First, let us estimate $G(s)$ from (4.2). To begin with, we expand the products $t^{-1}K_0(t)\mathcal{R}(t)$ and $t^{-1}I_0(t)\mathcal{R}(t)$ for a small argument $t \ll 1$:

$$
\begin{aligned}
t^{-1}I_0(t)\mathcal{R}(t) \;\simeq\; & p_1\, t^{-3} \,+\, p_2\, t^{-1} \log t \,+\, \left(\frac{p_1}{4} + p_3\right) t^{-1} \\
& +\, \left(p_4 \log^2 t \,+\, \left(\frac{p_2}{4} + p_5\right) \log t \,+\, \widehat{k}\right) t \,+\, \ldots;
\end{aligned}
\tag{A1}
$$

$$
\begin{aligned}
t^{-1}K_0(t)\mathcal{R}(t) \;\simeq\; & -p_1 \log\!\left(\frac{\gamma}{2}\,t\right) t^{-3} \,-\, \left(p_2 \log^2 t \,+\, k_1 \log t \,+\, k_2\right) t^{-1} \\
& -\, \left(p_4 \log^3 t \,+\, k_3 \log^2 t \,+\, k_4 \log t \,+\, k_5\right) t \,+\, \ldots,
\end{aligned}
\tag{A2}
$$

where $p_1, p_2, \ldots, p_5$ are given by (3.32), and the coefficients k_1, k_2, and k_3 are expressed as follows:

$$
\begin{aligned}
k_1 &= \frac{p_1}{4} + \log\!\left(\frac{\gamma}{2}\right) p_2 + p_3, \\
k_2 &= -\frac{p_1}{4} + \log\!\left(\frac{\gamma}{2}\right) \left(\frac{p_1}{4} + p_3\right), \\
k_3 &= \frac{p_2}{4} + \log\!\left(\frac{\gamma}{2}\right) p_4 + p_5
\end{aligned}
\tag{A3}
$$

(γ is the Euler constant). The parameters k_4, k_5, and $\widehat{k}$ are not used in the present paper and can be found in [50].

---

[5]The author is grateful to M. Lazar for calling attention to [79] where the modified screw dislocation has also been obtained for the gauge Lagrangian of the Maxwell type.

Using (A1) and (A2), we obtain the following estimates for $s \ll 1$:

$$K_0(s)\left(B(\epsilon) - \int_\epsilon^s I_0(t)\mathcal{R}(t)\frac{dt}{t}\right)\Bigg|_{\epsilon\to 0} \simeq s^{-2}\left(\mathcal{K}_1 \log s + \mathcal{K}_2\right)$$

$$+ \sum_{i=0}^3 \mathcal{K}_{6-i}\log^i s + s^2\sum_{i=0}^3 \mathcal{K}_{10-i}\log^i s + \dots, \tag{A4}$$

where

$$\mathcal{K}_1 = \frac{-p_1}{2}, \qquad \mathcal{K}_2 = -\log\left(\frac{\gamma}{2}\right)\frac{p_1}{2}, \qquad \mathcal{K}_3 = \frac{p_2}{2}, \qquad \mathcal{K}_4 = \frac{p_1}{4} + \log\left(\frac{\gamma}{2}\right)\frac{p_2}{2} + p_3,$$

$$\mathcal{K}_5 = -\,\mathrm{const} + \left(\frac{3}{2} + \log\frac{\gamma}{2}\right)\frac{p_1}{4} + \log\left(\frac{\gamma}{2}\right)p_3,$$

$$\mathcal{K}_6 = -\,\mathrm{const}\times\log\frac{\gamma}{2} + \left(1 + 3\log\frac{\gamma}{2}\right)\frac{p_1}{8}, \qquad\qquad \mathcal{K}_7 = \frac{p_2}{8} + \frac{p_4}{2},$$

$$\mathcal{K}_8 = \frac{p_1}{16} + \log\left(\frac{\gamma}{2}\right)\frac{p_2}{8} + \frac{p_3}{4} - \left(1 - \log\frac{\gamma}{2}\right)\frac{p_4}{2} + \frac{p_5}{2}. \tag{A5}$$

Further, we get

$$I_0(s)\int_s^\infty K_0(t)\mathcal{R}(t)\frac{dt}{t} \simeq s^{-2}\left(\mathcal{I}_1\log s + \mathcal{I}_2\right)$$

$$+ \sum_{i=0}^3 \mathcal{I}_{6-i}\log^i s + s^2\sum_{i=0}^3 \mathcal{I}_{10-i}\log^i s + \dots, \tag{A6}$$

where

$$\mathcal{I}_1 = \frac{-p_1}{2}, \qquad \mathcal{I}_2 = -\left(1 + 2\log\frac{\gamma}{2}\right)\frac{p_1}{4}, \qquad \mathcal{I}_3 = \frac{p_2}{3}, \qquad \mathcal{I}_4 = \frac{k_1}{2},$$

$$\mathcal{I}_5 = \frac{-p_1}{8} + k_2, \qquad\qquad \mathcal{I}_6 = \mathcal{I}_K + \left(1 + 2\log\frac{\gamma}{2}\right)\frac{3p_1}{16}, \tag{A7}$$

$$\mathcal{I}_7 = \frac{p_2}{12} + \frac{p_4}{2}, \qquad\qquad \mathcal{I}_8 = \frac{k_1}{8} - \frac{3p_4}{4} + \frac{k_3}{2},$$

and k_1, k_2, and k_3 are given by (A3). The numerical constant $\mathcal{I}_K$ in $\mathcal{I}_6$ from (A7) implies the regularized value of the integral:

$$\mathcal{I}_K \equiv \int_1^\infty K_0(t)\mathcal{R}(t)\frac{dt}{t} + \int_0^1\left[K_0(t)\mathcal{R}(t) + p_1\log\left(\frac{\gamma}{2}t\right)t^{-2}\right.$$

$$\left. +\ k_2 + k_1\log t + p_2\log^2 t\right]\frac{dt}{t}. \tag{A8}$$

Finally, the series (4.3) is obtained by subtracting the series (A6) from (A4). The resulting coefficients (4.4) are calculated by means of (A5) and (A7): $q_i = \mathcal{K}_{i+1} - \mathcal{I}_{i+1}$ for $i = 1, 2, \dots, 7$. Since $\mathcal{K}_1 - \mathcal{I}_1 = 0$, the contribution $\propto s^{-2}\log s$ is absent in (4.3).

Appendix B

Now let us estimate $I_{\mathcal{F}}(\rho)$ from (4.6). First, we expand the products $t\, J_0(\mathcal{N}t)G(\kappa t)$ and $t\, \widetilde{Y}_0(\mathcal{N}t)G(\kappa t)$ for a small argument $t \ll 1$:

$$
\begin{aligned}
t\, J_0(\mathcal{N}t)\, G(\kappa t) \;\simeq\; & \frac{q_1}{\kappa^2}\, t^{-1} \;+\; t\left(q_2 \log^3(\mathcal{N}t) \right. \\
& \left. + \sum_{i=0}^{2} n_{3-i}\, \log^i(\mathcal{N}t) \right) + t^3 \sum_{i=0}^{3} n_{7-i}\, \log^i(\mathcal{N}t) \;+\; \dots,
\end{aligned}
\tag{B1}
$$

$$
\begin{aligned}
t\, \widetilde{Y}_0(\mathcal{N}t)\, G(\kappa t) \;\simeq\; & \frac{q_1}{\kappa^2}\, t^{-1} \log\!\left(\frac{\gamma}{2}\mathcal{N}t\right) \;+\; t\left(q_2 \log^4(\mathcal{N}t) \right. \\
& \left. + \sum_{i=0}^{3} m_{4-i}\, \log^i(\mathcal{N}t) \right) + t^3 \sum_{i=0}^{4} m_{9-i}\, \log^i(\mathcal{N}t) \;+\; \dots,
\end{aligned}
\tag{B2}
$$

where the parameters $n_1, n_2, \dots, n_5$ are expressed by means of the previously found coefficients (4.4):

$$
n_1 = 3 \log\!\left(\frac{\kappa}{\mathcal{N}}\right) q_2 \;+\; q_3\,,
$$

$$
n_2 = 3 \log^2\!\left(\frac{\kappa}{\mathcal{N}}\right) q_2 \;+\; 2 \log\!\left(\frac{\kappa}{\mathcal{N}}\right) q_3 \;+\; q_4\,,
$$

$$
n_3 = -\frac{\mathcal{N}^2}{\kappa^2}\frac{q_1}{4} \;+\; \log^3\!\left(\frac{\kappa}{\mathcal{N}}\right) q_2 \;+\; \log^2\!\left(\frac{\kappa}{\mathcal{N}}\right) q_3 \;+\; \log\!\left(\frac{\kappa}{\mathcal{N}}\right) q_4 \;+\; q_5\,,
\tag{B3}
$$

$$
n_4 = -\mathcal{N}^2 \frac{q_2}{4} \;+\; \kappa^2\, q_6\,,
$$

$$
n_5 = -\mathcal{N}^2 \frac{q_3}{4} \;+\; \kappa^2\, q_7 \;+\; 3 \log\!\left(\frac{\kappa}{\mathcal{N}}\right) n_4\,.
$$

The coefficients $m_1, m_2, \dots, m_6$ are expressed by means of $n_1, n_2, \dots, n_5$ and q_1 and q_2:

$$
m_1 = \log\!\left(\frac{\gamma}{2}\right) q_2 + n_1\,, \qquad m_2 = \log\!\left(\frac{\gamma}{2}\right) n_1 + n_2\,,
$$

$$
m_3 = \log\!\left(\frac{\gamma}{2}\right) n_2 + n_3\,, \qquad m_4 = \frac{\mathcal{N}^2}{\kappa^2}\frac{q_1}{4} + \log\!\left(\frac{\gamma}{2}\right) n_3\,,
\tag{B4}
$$

$$
m_5 = n_4\,, \qquad\qquad m_6 = \mathcal{N}^2 \frac{q_2}{4} + \log\!\left(\frac{\gamma}{2}\right) n_4 + n_5\,.
$$

The coefficients n_6 and n_7, and m_7, m_8, and m_9 are present in (B1) and (B2) only formally: their explicit values are not of importance for the present investigation.

Using (B1)–(B4), we estimate the integrals that constitute $I_{\mathcal{F}}(\rho)$ and obtain

$$
\begin{aligned}
I_{\mathcal{F}}(\rho) \;\simeq\; & f_0 \;+\; f_1 \log^2(\mathcal{N}\rho) \;+\; f_2 \log(\mathcal{N}\rho) \\
& + \rho^2 \sum_{i=0}^{3} f_{7-i}\, \log^i(\mathcal{N}\rho) \;+\; \rho^4 f_9 \log^3(\mathcal{N}\rho) \;+\; \dots,
\end{aligned}
\tag{B5}
$$

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where

$$f_0 = \log\left(\frac{\gamma}{2}\right)\mathcal{I}_J - \mathcal{I}_Y, \qquad f_1 = \frac{q_1}{2\kappa^2}, \qquad f_2 = \mathcal{I}_J, \qquad f_4 = \frac{q_2}{4},$$

$$f_5 = -\frac{\mathcal{N}^2}{\kappa^2}\frac{q_1}{8} + \log\left(\frac{\gamma}{2}\right)\frac{n_2}{2} + \left(1 - \log\frac{\gamma}{2}\right)\widehat{\mathcal{Y}}_1 - \widehat{\mathcal{J}}_1,$$

$$f_6 = \frac{\mathcal{N}^2}{4}\left(-\mathcal{I}_J + \frac{q_1}{\kappa^2}\right) + \log\left(\frac{\gamma}{2}\right)\widehat{\mathcal{Y}}_1 + \widehat{\mathcal{Y}}_2 - \widehat{\mathcal{J}}_2, \tag{B6}$$

$$f_7 = \frac{\mathcal{N}^2}{4}\left(\mathcal{I}_Y + \left(1 - \log\frac{\gamma}{2}\right)\mathcal{I}_J\right) + \log\left(\frac{\gamma}{2}\right)\widehat{\mathcal{Y}}_2 - \widehat{\mathcal{J}}_3, \qquad f_9 = \frac{n_4}{16}.$$

The following notation is accepted in (B6):

$$\widehat{\mathcal{Y}}_1 = \frac{3q_2}{4} + \frac{n_2 - n_1}{2}, \qquad \widehat{\mathcal{Y}}_2 = -\frac{\widehat{\mathcal{Y}}_1}{2} + \frac{n_3}{2}, \tag{B7}$$

$$\widehat{\mathcal{J}}_1 = \frac{3q_2}{2} - \frac{3m_1}{4} + \frac{m_2}{2}, \qquad \widehat{\mathcal{J}}_2 = -\widehat{\mathcal{J}}_1 + \frac{m_3}{2}, \qquad \widehat{\mathcal{J}}_3 = -\frac{\widehat{\mathcal{J}}_2}{2} + \frac{m_4}{2}. \tag{B8}$$

In addition, we denote

$$\mathcal{I}_J \equiv \widetilde{\mathcal{I}}_J - \frac{q_1}{\kappa^2}\log\mathcal{N},$$

$$\mathcal{I}_Y \equiv \widetilde{\mathcal{I}}_Y - \frac{q_1}{\kappa^2}\log\mathcal{N}\left(\frac{\log\mathcal{N}}{2} + \log\frac{\gamma}{2}\right), \tag{B9}$$

where

$$\widetilde{\mathcal{I}}_J \equiv \lim_{\epsilon\to0+}\left(-\int_\epsilon^\infty J_0(\mathcal{N}t)\,G(\kappa t)\,t\,dt + \frac{q_1}{\kappa^2}\int_\epsilon^1 \frac{dt}{t}\right),$$

$$\widetilde{\mathcal{I}}_Y \equiv \lim_{\epsilon\to0+}\left(-\int_\epsilon^\infty \widetilde{Y}_0(\mathcal{N}t)\,G(\kappa t)\,t\,dt + \frac{q_1}{\kappa^2}\int_\epsilon^1 \log\left(\frac{\gamma}{2}\mathcal{N}t\right)\frac{dt}{t}\right). \tag{B10}$$

It should be pointed out that possible contributions $\propto \log^4(\mathcal{N}\rho)$ are cancelled in (B5): for instance, the coincidence of the coefficients n_4 and m_5 (see (B4)) results in the absence of the corresponding term of the fourth degree in ρ. Moreover, n_5 (B3) and m_6 (B4) are necessary to calculate f_9 (B6).

Eventually, the estimate (4.7) appears after re-arrangement of (B5). Generally, the corresponding coefficients $r_0, r_1, \ldots, r_7$ look as follows:

$$r_0 = f_0 + f_1\log^2\mathcal{N} + f_2\log\mathcal{N}, \qquad r_1 = 2f_1\log\mathcal{N} + f_2,$$

$$r_2 = f_1, \qquad r_3 = f_4, \qquad r_4 = 3f_4\log\mathcal{N} + f_5,$$

$$r_5 = 3f_4\log^2\mathcal{N} + 2f_5\log\mathcal{N} + f_6, \tag{B11}$$

$$r_6 = f_4\log^3\mathcal{N} + f_5\log^2\mathcal{N} + f_6\log\mathcal{N} + f_7,$$

$$r_7 = f_9 = (\kappa^2 - \mathcal{N}^2)\frac{p_2}{384}.$$

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We obtain r_0, r_1, r_2, and r_3 by means of (B6). To obtain r_4 (4.8), we re-express f_5:

$$f_5 = \left(1 - \frac{\mathcal{N}^2}{\kappa^2}\right)\frac{p_1}{32} - \left(1 + \log\frac{\mathcal{N}}{\kappa}\right)\frac{p_2}{8} + \frac{p_3}{8}. \tag{B12}$$

Now we turn to r_5 and r_6 from (5.10). Although f_6 and f_7 are left undone, their dependence on *const* can be extracted by means of (B6)–(B10) as follows:

$$f_6 = -\kappa^2\frac{\widetilde{C}}{4k} + \dots, \qquad f_7 = \kappa^2(q + \log\mathcal{N})\frac{\widetilde{C}}{4k} + \dots, \tag{B13}$$

where $\widetilde{C}$ and q are determined by (5.11). Since f_4 (B6) and f_5 (B12) are free from *const*, the equation (5.10) is indeed valid.

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